



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 10:13 AM EDT

PDB ID : 6PZW
EMDB ID : EMD-20538
Title : CryoEM derived model of NA-22 Fab in complex with N9 Shanghai2
Authors : Ward, A.B.; Turner, H.L.; Zhu, X.
Deposited on : 2019-08-01
Resolution : 3.00 Å (reported)
Based on initial model : 5L14

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

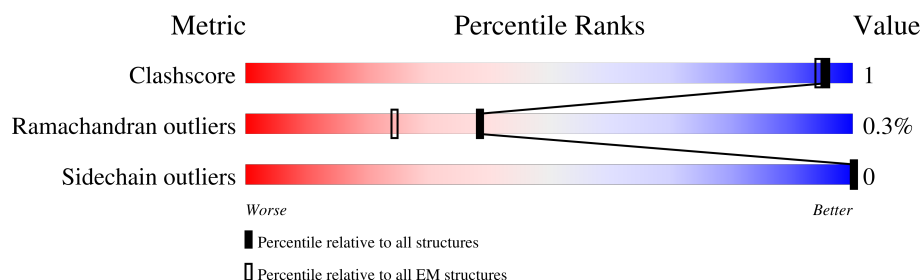
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	84% 6% 10%
1	B	429	84% 6% 10%
1	C	429	85% 6% 10%
1	D	429	84% 6% 10%
2	E	216	49% 50%
2	G	216	49% 50%
2	I	216	49% 50%
2	L	216	49% 50%

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Mol	Chain	Length	Quality of chain
3	F	227	
3	H	227	
3	J	227	
3	K	227	
4	M	2	
4	O	2	
4	Q	2	
4	T	2	
5	N	9	
5	P	9	
5	R	9	
5	S	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19778 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		
1	D	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		
1	C	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		
1	B	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		

- Molecule 2 is a protein called NA-22 fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	108	Total	C	N	O	S	0	0
			790	485	133	169	3		
2	E	108	Total	C	N	O	S	0	0
			790	485	133	169	3		
2	G	108	Total	C	N	O	S	0	0
			790	485	133	169	3		
2	L	108	Total	C	N	O	S	0	0
			790	485	133	169	3		

- Molecule 3 is a protein called NA-22 fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	122	Total	C	N	O	S	0	0
			957	609	166	177	5		
3	F	122	Total	C	N	O	S	0	0
			957	609	166	177	5		
3	J	122	Total	C	N	O	S	0	0
			957	609	166	177	5		
3	H	122	Total	C	N	O	S	0	0
			957	609	166	177	5		

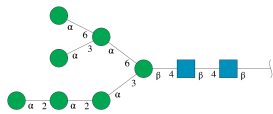
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	9	Total	C	N	O	0	0
			105	58	2	45		
5	P	9	Total	C	N	O	0	0
			105	58	2	45		
5	R	9	Total	C	N	O	0	0
			105	58	2	45		
5	S	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

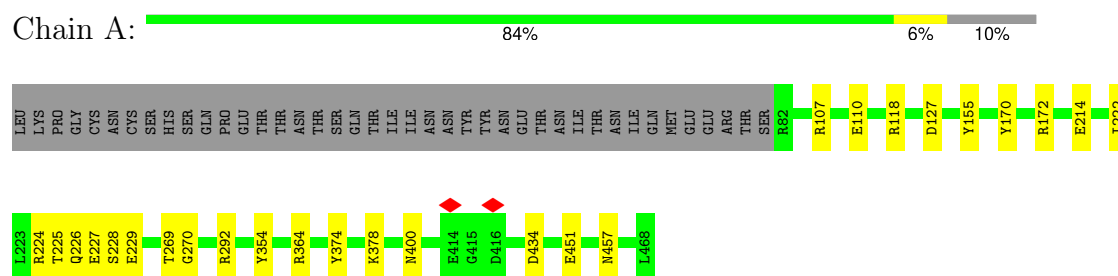


Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

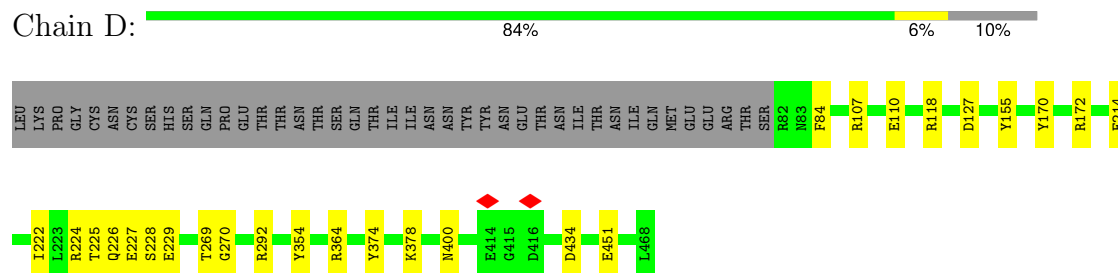
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

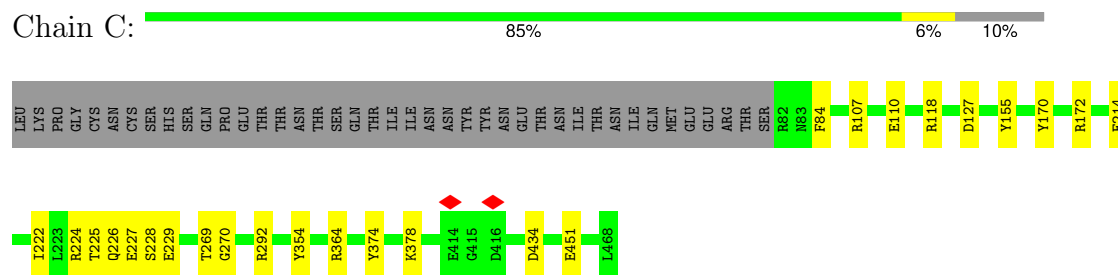
• Molecule 1: Neuraminidase



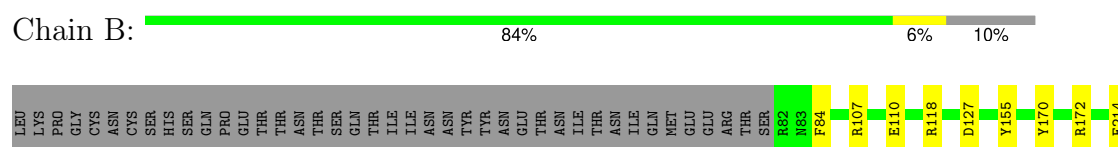
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase

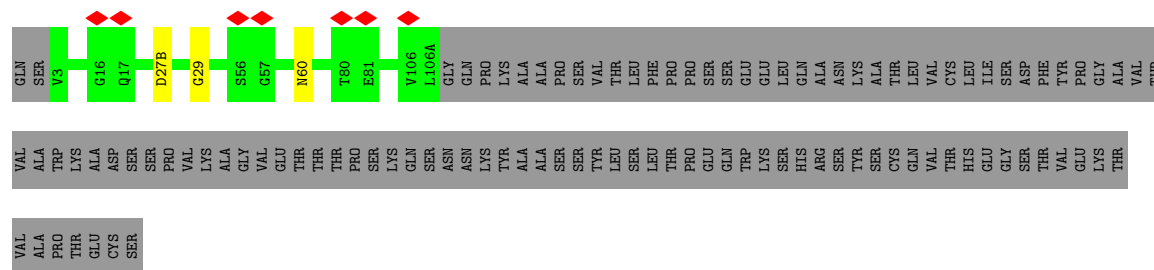


• Molecule 1: Neuraminidase

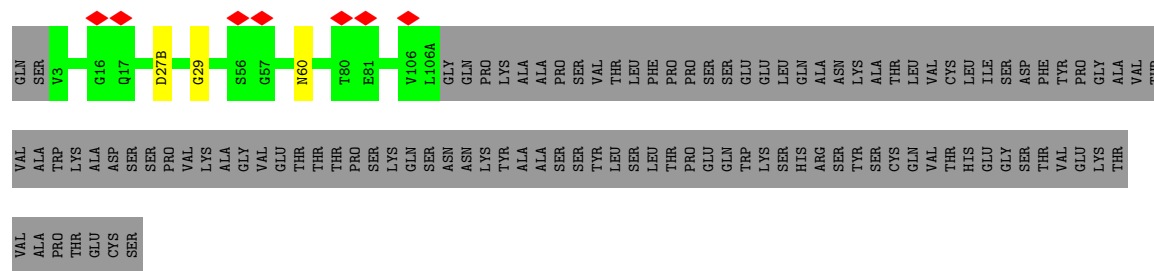




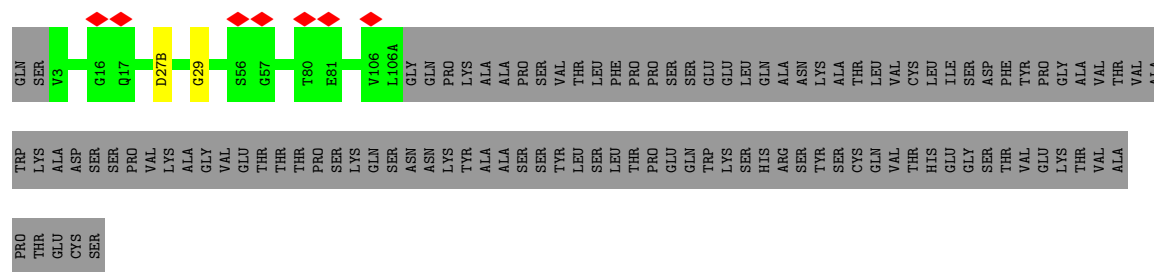
- Molecule 2: NA-22 fragment antigen binding light chain



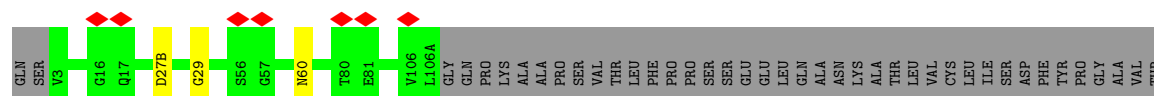
- Molecule 2: NA-22 fragment antigen binding light chain



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- Molecule 2: NA-22 fragment antigen binding light chain



VAL	ALA	TRP	LYS	ALA	ASP	SER	SER	PRO	VAL	LYS	GLY	ALA	VAL	GLU	THR	THR	PRO	LYS	GLN	SER	ASN	ASN	LYS	TYR	ALA	ALA	SER	SER	TYR	LEU	LEU	THR	PRO	GLU	GLN	THR	LYS	SER	HIS	ARG	SER	TYR	THR	SER	CYS	GLN	VAL	THR	THR	HIS	GLU	SER	THR	VAL	GLU	LYS	THR
VAL	ALA	PRO	THR	GLU	CYS	SER																																																			

- Molecule 3: NA-22 fragment antigen binding heavy chain

Chain K:  52% 46%

PRO	LYS	SER	CYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
SER	TRP	ASN	SER	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	ALA	VAL	LEU	GLN	SER	SER	GLY	LEU	TYR	SER	THR	LEU	SER	SER	VAL	VAL	THR	VAL	PRO	PRO	SER	SER	SER	LEU	GLY	THR	GLN	THR	TYR	TLE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASN	THR	LYS	VAL	ASP	LYS	ARG	VAL	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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- Molecule 3: NA-22 fragment antigen binding heavy chain

Chain F:  52% 46%

Q1	R16	G42	W47	F67	R71	E85	I99	Q105	V111	SER	GLY	ALA	THR	LYS	GLY	SER	PRO	SER	VAL	VAL	THR	VAL	PRO	PHE	PRO	LEU	SER	ALA	PRO	SER	GLY	THR	THR	LYS	THR	GLY	THR	ASN	VAL	ASN	HIS	GLY	CYS	VAL	LEU	ASN	LYS	THR	ASP	THR	PHE	PRO	GLU	PRO	VAL	THR	VAL
PRO	LYS	SER	CYS																																																						

- Molecule 3: NA-22 fragment antigen binding heavy chain

Chain J:  52% 46%

Q1	R16	G42	W47	F67	R71	E85	I99	Q105	V111	SER	GLY	ALA	THR	LYS	GLY	SER	PRO	SER	VAL	VAL	THR	VAL	PRO	PHE	PRO	LEU	SER	ALA	PRO	SER	GLY	THR	THR	LYS	THR	GLY	THR	ASN	VAL	ASN	HIS	GLY	CYS	VAL	LEU	ASN	LYS	THR	ASP	THR	PHE	PRO	GLU	PRO	VAL	THR	VAL
PRO	LYS	SER	CYS																																																						

- Molecule 3: NA-22 fragment antigen binding heavy chain

Chain H:  52% 46%

Q1	R16	G42	W47	F67	R71	E85	I99	Q105	V111	SER	GLY	ALA	THR	LYS	GLY	SER	PRO	SER	VAL	VAL	THR	VAL	PRO	PHE	PRO	LEU	SER	ALA	PRO	SER	GLY	THR	THR	LYS	THR	GLY	THR	ASN	VAL	ASN	HIS	GLY	CYS	VAL	LEU	ASN	LYS	THR	ASP	THR	PHE	PRO	GLU	PRO	VAL	THR	VAL
PRO	LYS	SER	CYS																																																						

SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS ARG VAL GLU

PRO
LYS
SER
CYS

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



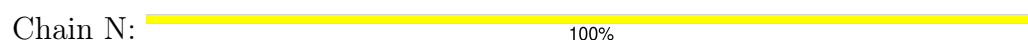
NAG1
NAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	20922	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.286	Depositor
Minimum map value	-2.437	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.143	Depositor
Recommended contour level	0.985	Depositor
Map size (\AA)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.14	11/3136 (0.4%)	0.94	9/4271 (0.2%)
1	B	1.14	11/3136 (0.4%)	0.94	9/4271 (0.2%)
1	C	1.14	11/3136 (0.4%)	0.94	9/4271 (0.2%)
1	D	1.14	11/3136 (0.4%)	0.94	9/4271 (0.2%)
2	E	0.95	0/806	0.87	2/1098 (0.2%)
2	G	0.95	0/806	0.87	2/1098 (0.2%)
2	I	0.95	0/806	0.87	2/1098 (0.2%)
2	L	0.95	0/806	0.87	2/1098 (0.2%)
3	F	1.05	1/979 (0.1%)	0.95	3/1325 (0.2%)
3	H	1.05	1/979 (0.1%)	0.95	3/1325 (0.2%)
3	J	1.05	1/979 (0.1%)	0.95	3/1325 (0.2%)
3	K	1.05	1/979 (0.1%)	0.95	3/1325 (0.2%)
All	All	1.09	48/19684 (0.2%)	0.93	56/26776 (0.2%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	TYR	CE2-CZ	-6.25	1.30	1.38
1	D	170	TYR	CE2-CZ	-6.25	1.30	1.38
1	C	170	TYR	CE2-CZ	-6.25	1.30	1.38
1	B	170	TYR	CE2-CZ	-6.25	1.30	1.38
1	A	155	TYR	CB-CG	-6.21	1.42	1.51
1	D	155	TYR	CB-CG	-6.21	1.42	1.51
1	C	155	TYR	CB-CG	-6.21	1.42	1.51
1	B	155	TYR	CB-CG	-6.21	1.42	1.51
1	A	155	TYR	CG-CD2	-5.76	1.31	1.39
1	D	155	TYR	CG-CD2	-5.76	1.31	1.39
1	C	155	TYR	CG-CD2	-5.76	1.31	1.39
1	B	155	TYR	CG-CD2	-5.76	1.31	1.39
1	A	227	GLU	CD-OE1	-5.63	1.19	1.25
1	D	227	GLU	CD-OE1	-5.63	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	GLU	CD-OE1	-5.63	1.19	1.25
1	B	227	GLU	CD-OE1	-5.63	1.19	1.25
1	A	451	GLU	CD-OE2	-5.38	1.19	1.25
1	D	451	GLU	CD-OE2	-5.38	1.19	1.25
1	C	451	GLU	CD-OE2	-5.38	1.19	1.25
1	B	451	GLU	CD-OE2	-5.38	1.19	1.25
1	A	227	GLU	CG-CD	-5.17	1.44	1.51
1	D	227	GLU	CG-CD	-5.17	1.44	1.51
1	C	227	GLU	CG-CD	-5.17	1.44	1.51
1	B	227	GLU	CG-CD	-5.17	1.44	1.51
1	A	155	TYR	CD2-CE2	-5.14	1.31	1.39
1	D	155	TYR	CD2-CE2	-5.14	1.31	1.39
1	C	155	TYR	CD2-CE2	-5.14	1.31	1.39
1	B	155	TYR	CD2-CE2	-5.14	1.31	1.39
1	A	110	GLU	CD-OE2	-5.12	1.20	1.25
1	D	110	GLU	CD-OE2	-5.12	1.20	1.25
1	C	110	GLU	CD-OE2	-5.12	1.20	1.25
1	B	110	GLU	CD-OE2	-5.12	1.20	1.25
1	A	354	TYR	CD2-CE2	-5.09	1.31	1.39
1	D	354	TYR	CD2-CE2	-5.09	1.31	1.39
1	C	354	TYR	CD2-CE2	-5.09	1.31	1.39
1	B	354	TYR	CD2-CE2	-5.09	1.31	1.39
1	A	214	GLU	CD-OE1	-5.08	1.20	1.25
1	D	214	GLU	CD-OE1	-5.08	1.20	1.25
1	C	214	GLU	CD-OE1	-5.08	1.20	1.25
1	B	214	GLU	CD-OE1	-5.08	1.20	1.25
3	K	47	TRP	CD2-CE2	-5.06	1.35	1.41
3	F	47	TRP	CD2-CE2	-5.06	1.35	1.41
3	J	47	TRP	CD2-CE2	-5.06	1.35	1.41
3	H	47	TRP	CD2-CE2	-5.06	1.35	1.41
1	A	214	GLU	CD-OE2	-5.02	1.20	1.25
1	D	214	GLU	CD-OE2	-5.02	1.20	1.25
1	C	214	GLU	CD-OE2	-5.02	1.20	1.25
1	B	214	GLU	CD-OE2	-5.02	1.20	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	D	118	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	C	118	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	B	118	ARG	NE-CZ-NH2	-10.14	115.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	71	ARG	NE-CZ-NH2	-8.88	115.86	120.30
3	F	71	ARG	NE-CZ-NH2	-8.88	115.86	120.30
3	J	71	ARG	NE-CZ-NH2	-8.88	115.86	120.30
3	H	71	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	172	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	D	172	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	C	172	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	172	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	364	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	D	364	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	364	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	364	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	224	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	224	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	224	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	224	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	I	27(B)	ASP	CB-CG-OD2	-6.90	112.09	118.30
2	E	27(B)	ASP	CB-CG-OD2	-6.90	112.09	118.30
2	G	27(B)	ASP	CB-CG-OD2	-6.90	112.09	118.30
2	L	27(B)	ASP	CB-CG-OD2	-6.90	112.09	118.30
2	I	27(B)	ASP	CB-CG-OD1	6.44	124.10	118.30
2	E	27(B)	ASP	CB-CG-OD1	6.44	124.10	118.30
2	G	27(B)	ASP	CB-CG-OD1	6.44	124.10	118.30
2	L	27(B)	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	107	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	107	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	107	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	107	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	354	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	D	354	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	C	354	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	B	354	TYR	CB-CG-CD2	-6.18	117.29	121.00
3	K	71	ARG	NE-CZ-NH1	5.85	123.22	120.30
3	F	71	ARG	NE-CZ-NH1	5.85	123.22	120.30
3	J	71	ARG	NE-CZ-NH1	5.85	123.22	120.30
3	H	71	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	374	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	D	374	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	C	374	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	B	374	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	A	292	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	292	ARG	NE-CZ-NH1	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	292	ARG	NE-CZ-NH1	5.29	122.95	120.30
3	K	67	PHE	CB-CG-CD1	5.18	124.43	120.80
3	F	67	PHE	CB-CG-CD1	5.18	124.43	120.80
3	J	67	PHE	CB-CG-CD1	5.18	124.43	120.80
3	H	67	PHE	CB-CG-CD1	5.18	124.43	120.80
1	A	118	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	D	118	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	C	118	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	B	118	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3054	0	2878	8	0
1	B	3054	0	2877	9	0
1	C	3054	0	2877	7	0
1	D	3054	0	2877	8	0
2	E	790	0	750	2	0
2	G	790	0	750	1	0
2	I	790	0	750	2	0
2	L	790	0	750	2	0
3	F	957	0	936	0	0
3	H	957	0	936	0	0
3	J	957	0	936	0	0
3	K	957	0	936	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
4	Q	28	0	25	0	0
4	T	28	0	25	0	0
5	N	105	0	83	0	0
5	P	105	0	83	0	0
5	R	105	0	83	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	105	0	83	0	0
6	B	14	0	13	1	0
6	C	14	0	13	1	0
6	D	14	0	13	1	0
All	All	19778	0	18724	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ASP:N	1:C:434:ASP:OD1	2.45	0.48
1:C:127:ASP:N	1:C:127:ASP:OD1	2.46	0.48
2:I:29:GLY:O	1:D:378:LYS:NZ	2.46	0.47
1:D:127:ASP:N	1:D:127:ASP:OD1	2.46	0.47
1:A:378:LYS:NZ	2:L:29:GLY:O	2.46	0.47
1:A:127:ASP:OD1	1:A:127:ASP:N	2.46	0.47
1:A:434:ASP:N	1:A:434:ASP:OD1	2.45	0.47
2:E:60:ASN:OD1	2:E:60:ASN:N	2.47	0.47
2:G:29:GLY:O	1:B:378:LYS:NZ	2.46	0.47
1:B:400:ASN:OD1	1:B:400:ASN:N	2.47	0.47
1:A:225:THR:OG1	1:A:226:GLN:N	2.47	0.47
1:D:434:ASP:OD1	1:D:434:ASP:N	2.45	0.47
1:C:225:THR:OG1	1:C:226:GLN:N	2.47	0.46
1:B:434:ASP:N	1:B:434:ASP:OD1	2.45	0.45
1:B:416:ASP:OD1	1:B:416:ASP:N	2.45	0.45
1:B:225:THR:OG1	1:B:226:GLN:N	2.47	0.45
1:A:400:ASN:OD1	1:A:400:ASN:N	2.47	0.45
1:B:127:ASP:OD1	1:B:127:ASP:N	2.46	0.44
2:I:60:ASN:N	2:I:60:ASN:OD1	2.47	0.44
2:E:29:GLY:O	1:C:378:LYS:NZ	2.46	0.44
1:D:225:THR:OG1	1:D:226:GLN:N	2.47	0.44
1:A:228:SER:OG	1:A:229:GLU:N	2.51	0.43
1:B:228:SER:OG	1:B:229:GLU:N	2.51	0.43
1:C:228:SER:OG	1:C:229:GLU:N	2.51	0.42
1:A:457:ASN:OD1	1:A:457:ASN:N	2.52	0.42
1:D:228:SER:OG	1:D:229:GLU:N	2.51	0.42
1:D:269:THR:OG1	1:D:270:GLY:N	2.53	0.42
1:C:84:PHE:O	6:C:1301:NAG:H82	2.20	0.41
1:A:269:THR:OG1	1:A:270:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:THR:OG1	1:C:270:GLY:N	2.53	0.41
1:B:84:PHE:O	6:B:1301:NAG:H82	2.20	0.41
1:B:269:THR:OG1	1:B:270:GLY:N	2.53	0.41
2:L:60:ASN:OD1	2:L:60:ASN:N	2.47	0.41
1:D:84:PHE:O	6:D:1301:NAG:H82	2.20	0.41
1:D:400:ASN:OD1	1:D:400:ASN:N	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/429 (90%)	375 (97%)	10 (3%)	1 (0%)	37	70
1	B	386/429 (90%)	375 (97%)	10 (3%)	1 (0%)	37	70
1	C	386/429 (90%)	375 (97%)	10 (3%)	1 (0%)	37	70
1	D	386/429 (90%)	375 (97%)	10 (3%)	1 (0%)	37	70
2	E	106/216 (49%)	103 (97%)	3 (3%)	0	100	100
2	G	106/216 (49%)	103 (97%)	3 (3%)	0	100	100
2	I	106/216 (49%)	103 (97%)	3 (3%)	0	100	100
2	L	106/216 (49%)	103 (97%)	3 (3%)	0	100	100
3	F	120/227 (53%)	119 (99%)	0	1 (1%)	16	51
3	H	120/227 (53%)	119 (99%)	0	1 (1%)	16	51
3	J	120/227 (53%)	119 (99%)	0	1 (1%)	16	51
3	K	120/227 (53%)	119 (99%)	0	1 (1%)	16	51
All	All	2448/3488 (70%)	2388 (98%)	52 (2%)	8 (0%)	38	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ILE
1	D	222	ILE
1	C	222	ILE
1	B	222	ILE
3	K	99	ILE
3	F	99	ILE
3	J	99	ILE
3	H	99	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/379 (89%)	339 (100%)	0	100	100
1	B	339/379 (89%)	339 (100%)	0	100	100
1	C	339/379 (89%)	339 (100%)	0	100	100
1	D	339/379 (89%)	339 (100%)	0	100	100
2	E	92/185 (50%)	92 (100%)	0	100	100
2	G	92/185 (50%)	92 (100%)	0	100	100
2	I	92/185 (50%)	92 (100%)	0	100	100
2	L	92/185 (50%)	92 (100%)	0	100	100
3	F	101/192 (53%)	101 (100%)	0	100	100
3	H	101/192 (53%)	101 (100%)	0	100	100
3	J	101/192 (53%)	101 (100%)	0	100	100
3	K	101/192 (53%)	101 (100%)	0	100	100
All	All	2128/3024 (70%)	2128 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

44 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	M	1	4,1	14,14,15	2.03	2 (14%)	17,19,21	1.04	2 (11%)
4	NAG	M	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.97	1 (5%)
5	NAG	N	1	5,1	14,14,15	1.86	2 (14%)	17,19,21	1.02	1 (5%)
5	NAG	N	2	5	14,14,15	2.02	3 (21%)	17,19,21	1.46	3 (17%)
5	BMA	N	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.12	1 (6%)
5	MAN	N	4	5	11,11,12	1.38	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	N	5	5	11,11,12	1.55	2 (18%)	15,15,17	1.01	2 (13%)
5	MAN	N	6	5	11,11,12	1.74	2 (18%)	15,15,17	0.97	0
5	MAN	N	7	5	11,11,12	1.85	2 (18%)	15,15,17	1.02	1 (6%)
5	MAN	N	8	5	11,11,12	1.79	2 (18%)	15,15,17	1.03	2 (13%)
5	MAN	N	9	5	11,11,12	1.80	2 (18%)	15,15,17	1.00	1 (6%)
4	NAG	O	1	4,1	14,14,15	2.03	2 (14%)	17,19,21	1.04	2 (11%)
4	NAG	O	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.97	1 (5%)
5	NAG	P	1	5,1	14,14,15	1.86	2 (14%)	17,19,21	1.02	1 (5%)
5	NAG	P	2	5	14,14,15	2.02	3 (21%)	17,19,21	1.46	3 (17%)
5	BMA	P	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.12	1 (6%)
5	MAN	P	4	5	11,11,12	1.38	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	P	5	5	11,11,12	1.55	2 (18%)	15,15,17	1.01	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	P	6	5	11,11,12	1.74	2 (18%)	15,15,17	0.97	0
5	MAN	P	7	5	11,11,12	1.85	2 (18%)	15,15,17	1.02	1 (6%)
5	MAN	P	8	5	11,11,12	1.79	2 (18%)	15,15,17	1.03	2 (13%)
5	MAN	P	9	5	11,11,12	1.80	2 (18%)	15,15,17	1.00	1 (6%)
4	NAG	Q	1	4,1	14,14,15	2.03	2 (14%)	17,19,21	1.04	2 (11%)
4	NAG	Q	2	4	14,14,15	2.09	2 (14%)	17,19,21	0.97	1 (5%)
5	NAG	R	1	5,1	14,14,15	1.86	2 (14%)	17,19,21	1.02	1 (5%)
5	NAG	R	2	5	14,14,15	2.02	3 (21%)	17,19,21	1.46	3 (17%)
5	BMA	R	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.12	1 (6%)
5	MAN	R	4	5	11,11,12	1.38	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	R	5	5	11,11,12	1.55	2 (18%)	15,15,17	1.01	2 (13%)
5	MAN	R	6	5	11,11,12	1.74	2 (18%)	15,15,17	0.97	0
5	MAN	R	7	5	11,11,12	1.85	2 (18%)	15,15,17	1.02	1 (6%)
5	MAN	R	8	5	11,11,12	1.79	2 (18%)	15,15,17	1.03	2 (13%)
5	MAN	R	9	5	11,11,12	1.80	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	S	1	5,1	14,14,15	1.86	2 (14%)	17,19,21	1.02	1 (5%)
5	NAG	S	2	5	14,14,15	2.02	3 (21%)	17,19,21	1.46	3 (17%)
5	BMA	S	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.12	1 (6%)
5	MAN	S	4	5	11,11,12	1.38	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	S	5	5	11,11,12	1.55	2 (18%)	15,15,17	1.01	2 (13%)
5	MAN	S	6	5	11,11,12	1.74	2 (18%)	15,15,17	0.97	0
5	MAN	S	7	5	11,11,12	1.85	2 (18%)	15,15,17	1.02	1 (6%)
5	MAN	S	8	5	11,11,12	1.79	2 (18%)	15,15,17	1.03	2 (13%)
5	MAN	S	9	5	11,11,12	1.80	2 (18%)	15,15,17	1.00	1 (6%)
4	NAG	T	1	4,1	14,14,15	0.38	0	17,19,21	0.70	0
4	NAG	T	2	4	14,14,15	0.39	0	17,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	2/2/19/22	0/1/1/1
5	MAN	N	5	5	-	1/2/19/22	0/1/1/1
5	MAN	N	6	5	-	2/2/19/22	0/1/1/1
5	MAN	N	7	5	-	2/2/19/22	0/1/1/1
5	MAN	N	8	5	-	1/2/19/22	0/1/1/1
5	MAN	N	9	5	-	1/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	2/2/19/22	0/1/1/1
5	MAN	P	5	5	-	1/2/19/22	0/1/1/1
5	MAN	P	6	5	-	2/2/19/22	0/1/1/1
5	MAN	P	7	5	-	2/2/19/22	0/1/1/1
5	MAN	P	8	5	-	1/2/19/22	0/1/1/1
5	MAN	P	9	5	-	1/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	R	2	5	-	1/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	2/2/19/22	0/1/1/1
5	MAN	R	5	5	-	1/2/19/22	0/1/1/1
5	MAN	R	6	5	-	2/2/19/22	0/1/1/1
5	MAN	R	7	5	-	2/2/19/22	0/1/1/1
5	MAN	R	8	5	-	1/2/19/22	0/1/1/1
5	MAN	R	9	5	-	1/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
5	BMA	S	3	5	-	2/2/19/22	0/1/1/1
5	MAN	S	4	5	-	2/2/19/22	0/1/1/1
5	MAN	S	5	5	-	1/2/19/22	0/1/1/1
5	MAN	S	6	5	-	2/2/19/22	0/1/1/1
5	MAN	S	7	5	-	2/2/19/22	0/1/1/1
5	MAN	S	8	5	-	1/2/19/22	0/1/1/1
5	MAN	S	9	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	2	NAG	O5-C1	6.55	1.54	1.43
4	O	2	NAG	O5-C1	6.55	1.54	1.43
4	Q	2	NAG	O5-C1	6.55	1.54	1.43
5	N	2	NAG	O5-C1	6.51	1.54	1.43
5	P	2	NAG	O5-C1	6.51	1.54	1.43
5	R	2	NAG	O5-C1	6.51	1.54	1.43
5	S	2	NAG	O5-C1	6.51	1.54	1.43
4	M	1	NAG	O5-C1	6.32	1.54	1.43
4	O	1	NAG	O5-C1	6.32	1.54	1.43
4	Q	1	NAG	O5-C1	6.32	1.54	1.43
5	N	1	NAG	O5-C1	5.64	1.53	1.43
5	P	1	NAG	O5-C1	5.64	1.53	1.43
5	R	1	NAG	O5-C1	5.64	1.53	1.43
5	S	1	NAG	O5-C1	5.64	1.53	1.43
5	N	8	MAN	O2-C2	-4.28	1.34	1.43
5	P	8	MAN	O2-C2	-4.28	1.34	1.43
5	R	8	MAN	O2-C2	-4.28	1.34	1.43
5	S	8	MAN	O2-C2	-4.28	1.34	1.43
5	N	3	BMA	O2-C2	-4.27	1.34	1.43
5	P	3	BMA	O2-C2	-4.27	1.34	1.43
5	R	3	BMA	O2-C2	-4.27	1.34	1.43
5	S	3	BMA	O2-C2	-4.27	1.34	1.43
5	N	7	MAN	O2-C2	-4.27	1.34	1.43
5	P	7	MAN	O2-C2	-4.27	1.34	1.43
5	R	7	MAN	O2-C2	-4.27	1.34	1.43
5	S	7	MAN	O2-C2	-4.27	1.34	1.43
5	N	9	MAN	O2-C2	-4.21	1.34	1.43
5	P	9	MAN	O2-C2	-4.21	1.34	1.43
5	R	9	MAN	O2-C2	-4.21	1.34	1.43
5	S	9	MAN	O2-C2	-4.21	1.34	1.43
5	N	6	MAN	O2-C2	-4.15	1.34	1.43
5	P	6	MAN	O2-C2	-4.15	1.34	1.43
5	R	6	MAN	O2-C2	-4.15	1.34	1.43
5	S	6	MAN	O2-C2	-4.15	1.34	1.43
5	N	5	MAN	O2-C2	-3.29	1.36	1.43
5	P	5	MAN	O2-C2	-3.29	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	5	MAN	O2-C2	-3.29	1.36	1.43
5	S	5	MAN	O2-C2	-3.29	1.36	1.43
5	N	4	MAN	O2-C2	-2.73	1.37	1.43
5	P	4	MAN	O2-C2	-2.73	1.37	1.43
5	R	4	MAN	O2-C2	-2.73	1.37	1.43
5	S	4	MAN	O2-C2	-2.73	1.37	1.43
5	N	6	MAN	C2-C3	-2.45	1.48	1.52
5	P	6	MAN	C2-C3	-2.45	1.48	1.52
5	R	6	MAN	C2-C3	-2.45	1.48	1.52
5	S	6	MAN	C2-C3	-2.45	1.48	1.52
4	M	1	NAG	C3-C2	-2.37	1.47	1.52
4	O	1	NAG	C3-C2	-2.37	1.47	1.52
4	Q	1	NAG	C3-C2	-2.37	1.47	1.52
5	N	9	MAN	C2-C3	-2.35	1.48	1.52
5	P	9	MAN	C2-C3	-2.35	1.48	1.52
5	R	9	MAN	C2-C3	-2.35	1.48	1.52
5	S	9	MAN	C2-C3	-2.35	1.48	1.52
5	N	3	BMA	C2-C3	-2.31	1.48	1.52
5	P	3	BMA	C2-C3	-2.31	1.48	1.52
5	R	3	BMA	C2-C3	-2.31	1.48	1.52
5	S	3	BMA	C2-C3	-2.31	1.48	1.52
5	N	8	MAN	C2-C3	-2.26	1.49	1.52
5	P	8	MAN	C2-C3	-2.26	1.49	1.52
5	R	8	MAN	C2-C3	-2.26	1.49	1.52
5	S	8	MAN	C2-C3	-2.26	1.49	1.52
5	N	1	NAG	C4-C3	2.21	1.58	1.52
5	P	1	NAG	C4-C3	2.21	1.58	1.52
5	R	1	NAG	C4-C3	2.21	1.58	1.52
5	S	1	NAG	C4-C3	2.21	1.58	1.52
5	N	7	MAN	C2-C3	-2.19	1.49	1.52
5	P	7	MAN	C2-C3	-2.19	1.49	1.52
5	R	7	MAN	C2-C3	-2.19	1.49	1.52
5	S	7	MAN	C2-C3	-2.19	1.49	1.52
5	N	2	NAG	C4-C3	2.19	1.58	1.52
5	P	2	NAG	C4-C3	2.19	1.58	1.52
5	R	2	NAG	C4-C3	2.19	1.58	1.52
5	S	2	NAG	C4-C3	2.19	1.58	1.52
4	M	2	NAG	C3-C2	-2.16	1.48	1.52
4	O	2	NAG	C3-C2	-2.16	1.48	1.52
4	Q	2	NAG	C3-C2	-2.16	1.48	1.52
5	N	5	MAN	C2-C3	-2.14	1.49	1.52
5	P	5	MAN	C2-C3	-2.14	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	5	MAN	C2-C3	-2.14	1.49	1.52
5	S	5	MAN	C2-C3	-2.14	1.49	1.52
5	N	2	NAG	C3-C2	-2.12	1.48	1.52
5	P	2	NAG	C3-C2	-2.12	1.48	1.52
5	R	2	NAG	C3-C2	-2.12	1.48	1.52
5	S	2	NAG	C3-C2	-2.12	1.48	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	2	NAG	C3-C4-C5	-4.02	102.95	110.23
5	P	2	NAG	C3-C4-C5	-4.02	102.95	110.23
5	R	2	NAG	C3-C4-C5	-4.02	102.95	110.23
5	S	2	NAG	C3-C4-C5	-4.02	102.95	110.23
4	M	2	NAG	C4-C3-C2	-2.96	106.68	111.02
4	O	2	NAG	C4-C3-C2	-2.96	106.68	111.02
4	Q	2	NAG	C4-C3-C2	-2.96	106.68	111.02
5	N	1	NAG	C3-C4-C5	-2.74	105.26	110.23
5	P	1	NAG	C3-C4-C5	-2.74	105.26	110.23
5	R	1	NAG	C3-C4-C5	-2.74	105.26	110.23
5	S	1	NAG	C3-C4-C5	-2.74	105.26	110.23
5	N	3	BMA	C2-C3-C4	-2.65	106.19	110.86
5	P	3	BMA	C2-C3-C4	-2.65	106.19	110.86
5	R	3	BMA	C2-C3-C4	-2.65	106.19	110.86
5	S	3	BMA	C2-C3-C4	-2.65	106.19	110.86
5	N	2	NAG	C1-O5-C5	-2.65	108.64	112.19
5	P	2	NAG	C1-O5-C5	-2.65	108.64	112.19
5	R	2	NAG	C1-O5-C5	-2.65	108.64	112.19
5	S	2	NAG	C1-O5-C5	-2.65	108.64	112.19
4	M	1	NAG	C1-O5-C5	-2.62	108.67	112.19
4	O	1	NAG	C1-O5-C5	-2.62	108.67	112.19
4	Q	1	NAG	C1-O5-C5	-2.62	108.67	112.19
5	N	2	NAG	C4-C3-C2	2.58	114.80	111.02
5	P	2	NAG	C4-C3-C2	2.58	114.80	111.02
5	R	2	NAG	C4-C3-C2	2.58	114.80	111.02
5	S	2	NAG	C4-C3-C2	2.58	114.80	111.02
5	N	7	MAN	C2-C3-C4	-2.52	106.42	110.86
5	P	7	MAN	C2-C3-C4	-2.52	106.42	110.86
5	R	7	MAN	C2-C3-C4	-2.52	106.42	110.86
5	S	7	MAN	C2-C3-C4	-2.52	106.42	110.86
5	N	4	MAN	O2-C2-C1	-2.50	103.49	109.22
5	P	4	MAN	O2-C2-C1	-2.50	103.49	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	4	MAN	O2-C2-C1	-2.50	103.49	109.22
5	S	4	MAN	O2-C2-C1	-2.50	103.49	109.22
5	N	9	MAN	C2-C3-C4	-2.37	106.69	110.86
5	P	9	MAN	C2-C3-C4	-2.37	106.69	110.86
5	R	9	MAN	C2-C3-C4	-2.37	106.69	110.86
5	S	9	MAN	C2-C3-C4	-2.37	106.69	110.86
4	M	1	NAG	C3-C4-C5	-2.16	106.32	110.23
4	O	1	NAG	C3-C4-C5	-2.16	106.32	110.23
4	Q	1	NAG	C3-C4-C5	-2.16	106.32	110.23
5	N	8	MAN	C2-C3-C4	-2.14	107.10	110.86
5	P	8	MAN	C2-C3-C4	-2.14	107.10	110.86
5	R	8	MAN	C2-C3-C4	-2.14	107.10	110.86
5	S	8	MAN	C2-C3-C4	-2.14	107.10	110.86
5	N	8	MAN	C1-C2-C3	2.14	112.76	109.64
5	P	8	MAN	C1-C2-C3	2.14	112.76	109.64
5	R	8	MAN	C1-C2-C3	2.14	112.76	109.64
5	S	8	MAN	C1-C2-C3	2.14	112.76	109.64
5	N	5	MAN	C2-C3-C4	-2.05	107.26	110.86
5	P	5	MAN	C2-C3-C4	-2.05	107.26	110.86
5	R	5	MAN	C2-C3-C4	-2.05	107.26	110.86
5	S	5	MAN	C2-C3-C4	-2.05	107.26	110.86
5	N	5	MAN	O2-C2-C1	-2.00	104.64	109.22
5	P	5	MAN	O2-C2-C1	-2.00	104.64	109.22
5	R	5	MAN	O2-C2-C1	-2.00	104.64	109.22
5	S	5	MAN	O2-C2-C1	-2.00	104.64	109.22

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
5	N	7	MAN	C4-C5-C6-O6
5	P	7	MAN	C4-C5-C6-O6
5	R	7	MAN	C4-C5-C6-O6
5	S	7	MAN	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
5	N	6	MAN	O5-C5-C6-O6
5	P	6	MAN	O5-C5-C6-O6
5	R	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	S	6	MAN	O5-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
5	P	4	MAN	O5-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6
5	S	4	MAN	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
5	N	7	MAN	O5-C5-C6-O6
5	P	7	MAN	O5-C5-C6-O6
5	R	7	MAN	O5-C5-C6-O6
5	S	7	MAN	O5-C5-C6-O6
5	N	6	MAN	C4-C5-C6-O6
5	P	6	MAN	C4-C5-C6-O6
5	R	6	MAN	C4-C5-C6-O6
5	S	6	MAN	C4-C5-C6-O6
5	N	8	MAN	O5-C5-C6-O6
5	N	9	MAN	O5-C5-C6-O6
5	P	8	MAN	O5-C5-C6-O6
5	P	9	MAN	O5-C5-C6-O6
5	R	8	MAN	O5-C5-C6-O6
5	R	9	MAN	O5-C5-C6-O6
5	S	8	MAN	O5-C5-C6-O6
5	S	9	MAN	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	N	5	MAN	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	P	5	MAN	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	R	5	MAN	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
5	S	5	MAN	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	N	4	MAN	C4-C5-C6-O6
5	P	4	MAN	C4-C5-C6-O6
5	R	4	MAN	C4-C5-C6-O6
5	S	4	MAN	C4-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6

Continued on next page...

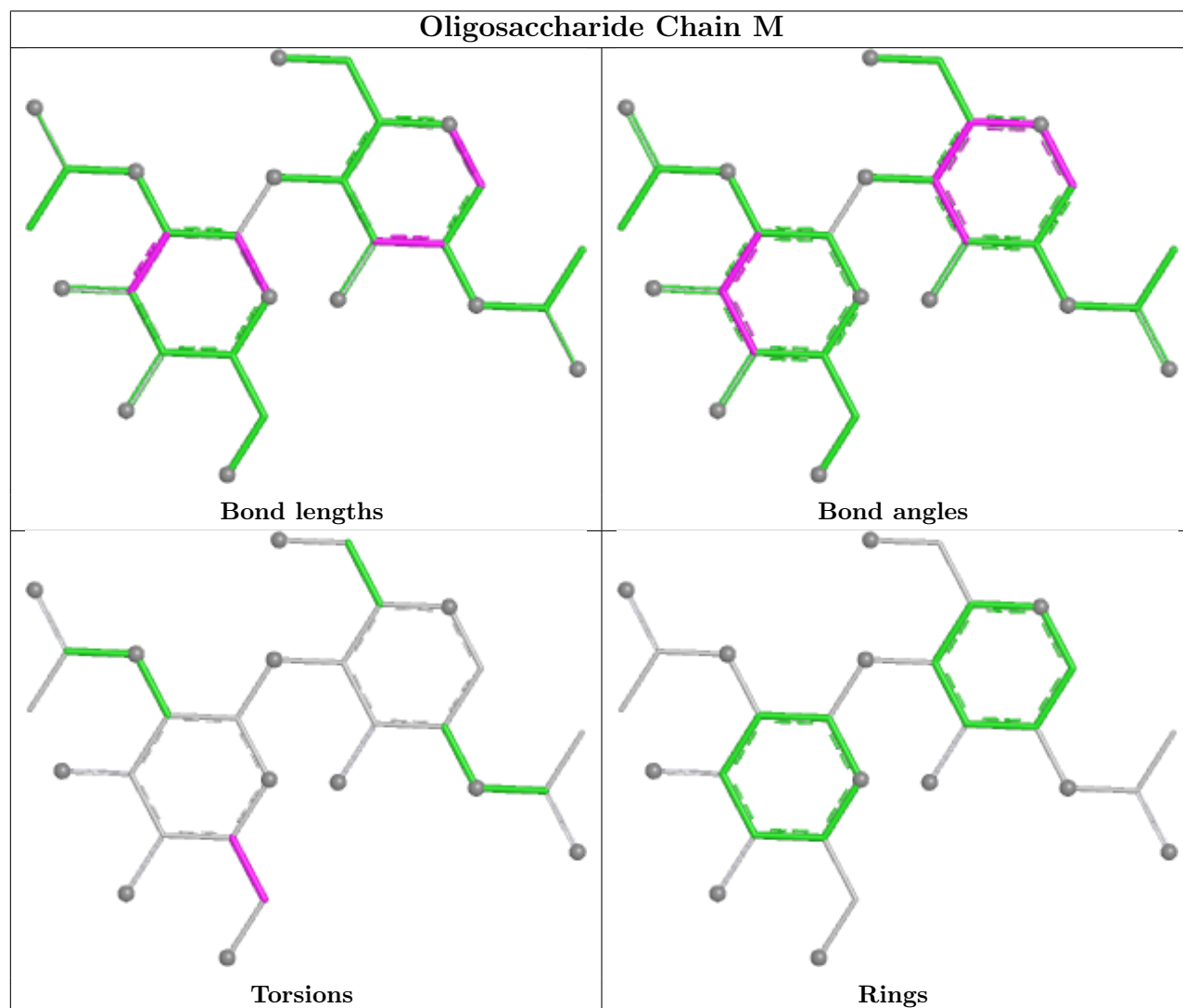
Continued from previous page...

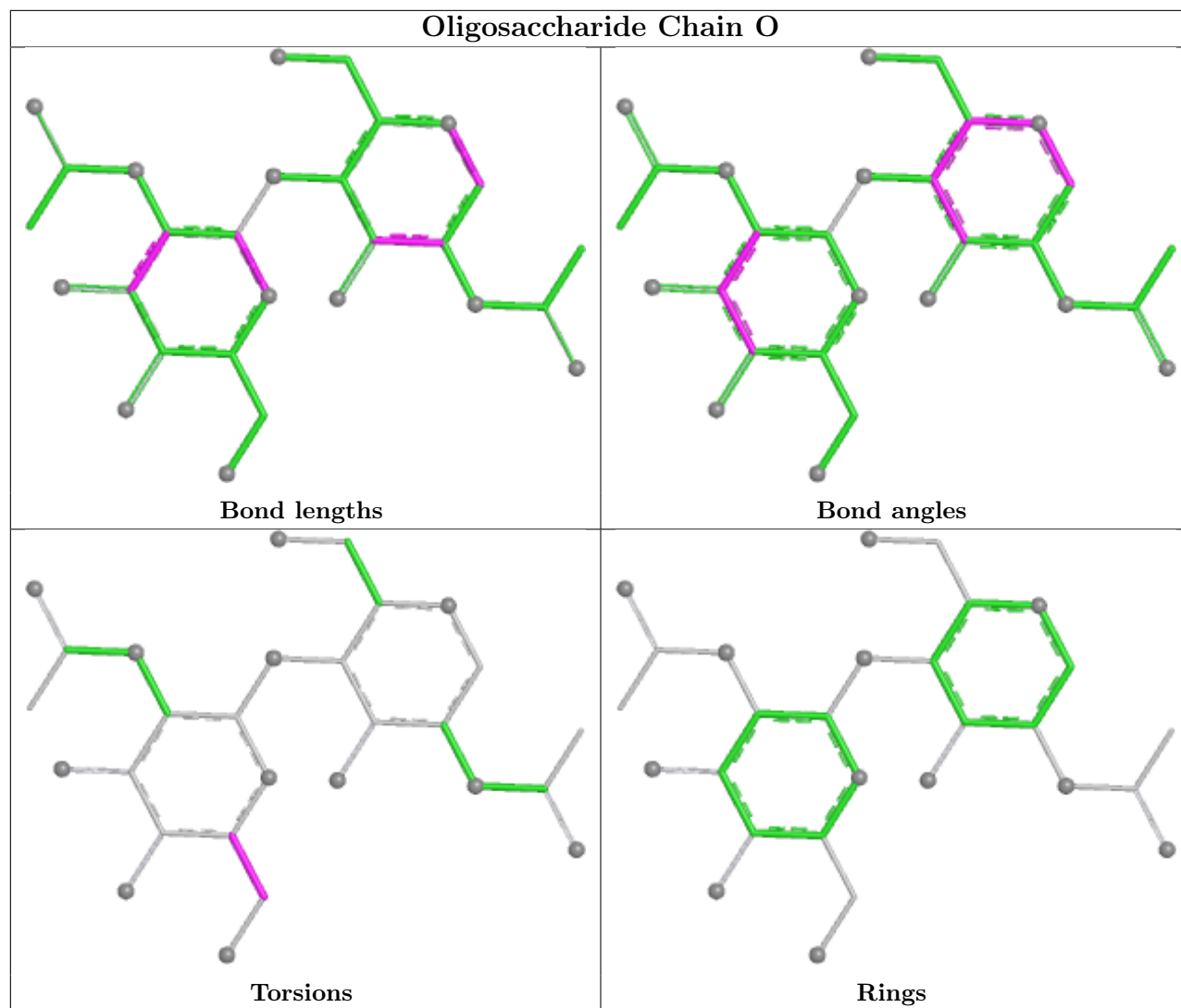
Mol	Chain	Res	Type	Atoms
5	R	3	BMA	C4-C5-C6-O6
5	S	3	BMA	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	S	3	BMA	O5-C5-C6-O6

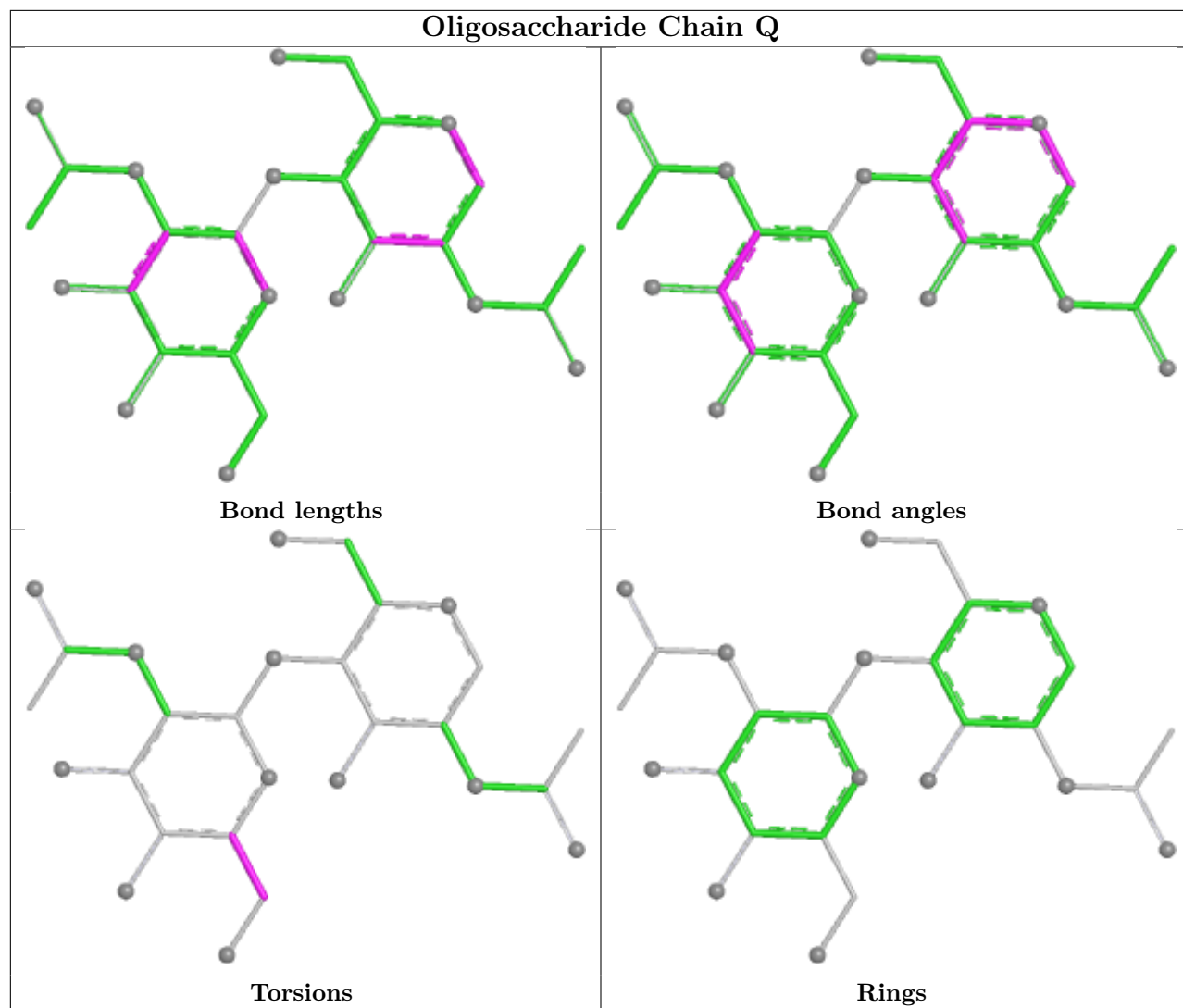
There are no ring outliers.

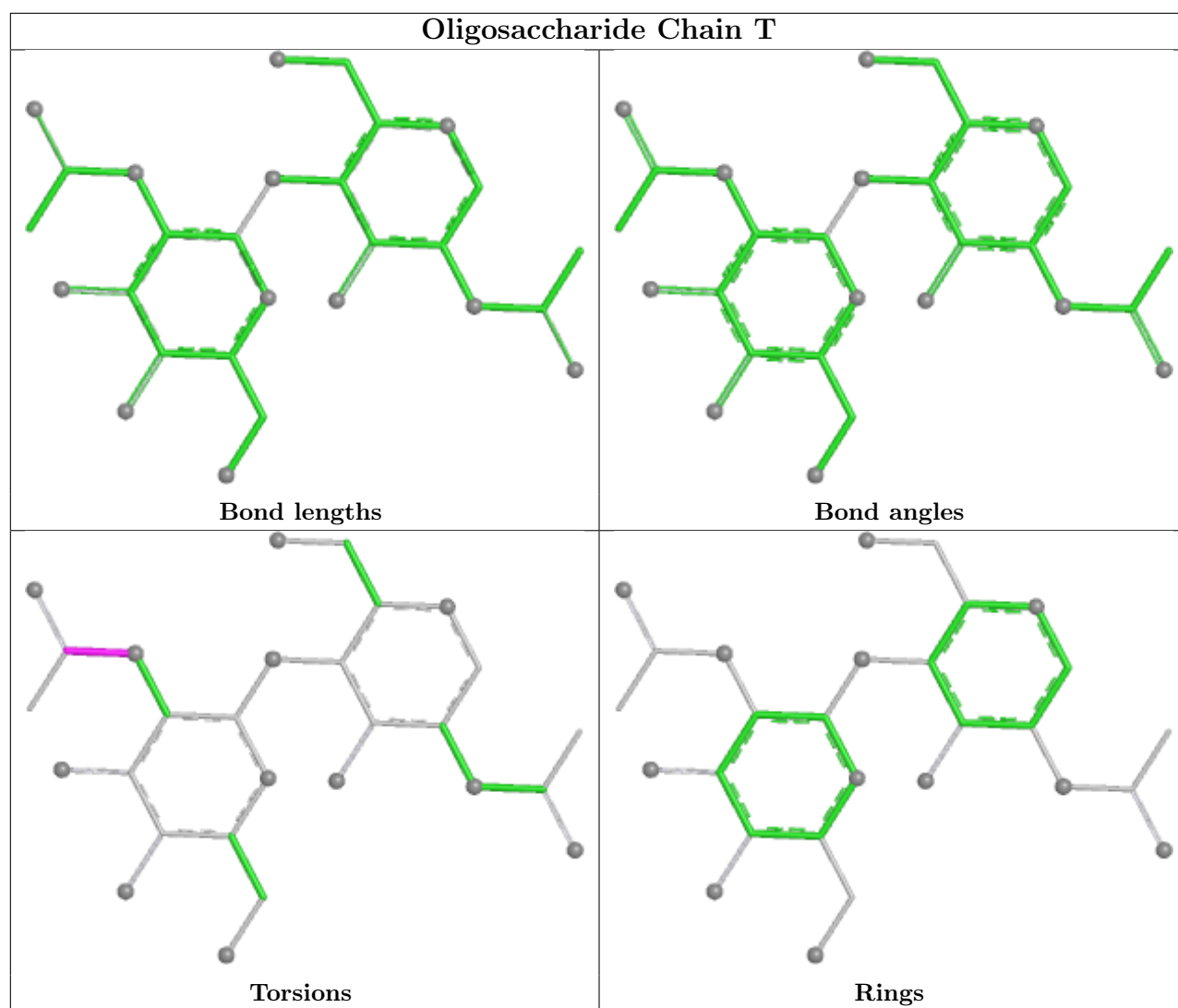
No monomer is involved in short contacts.

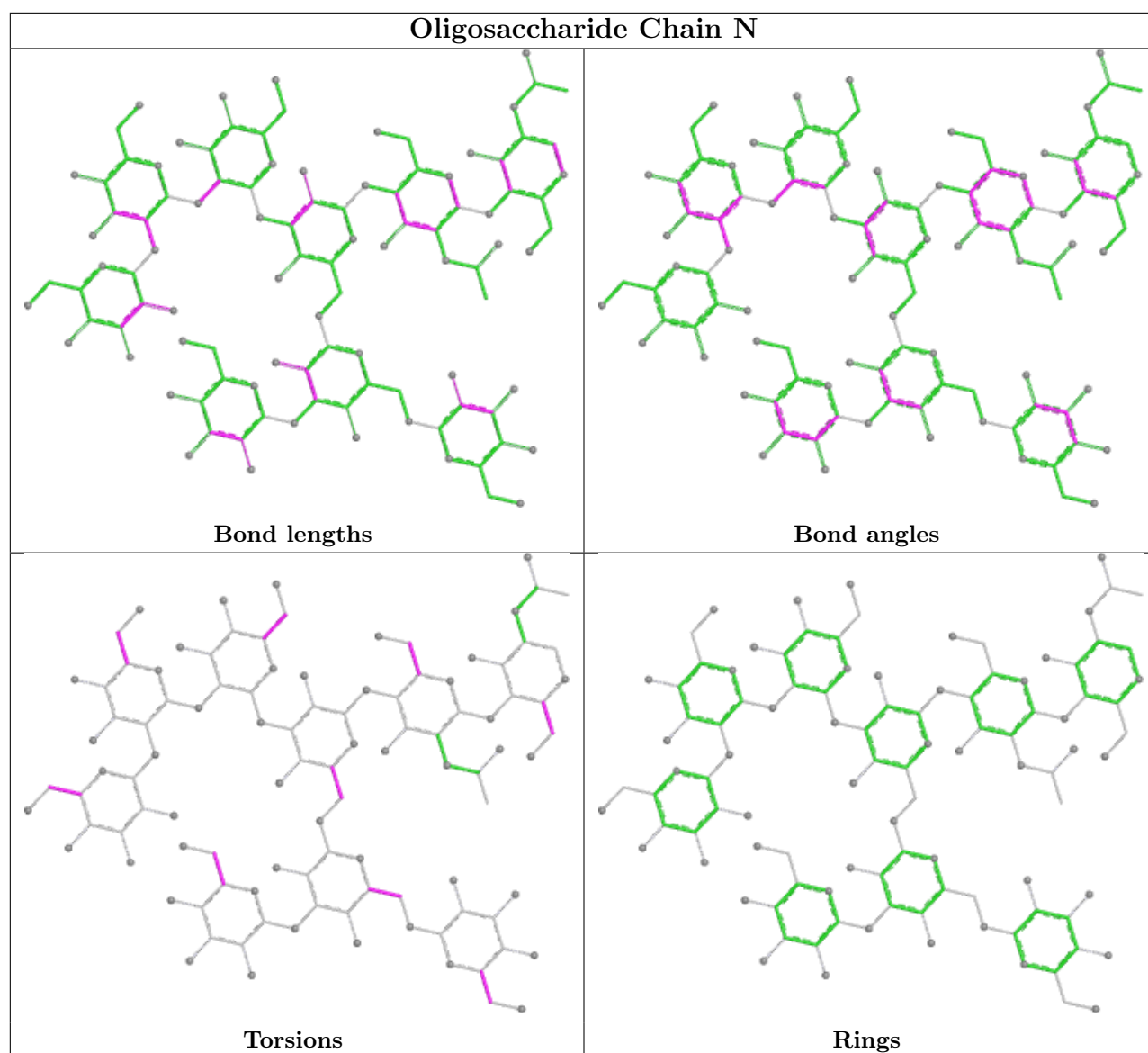
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

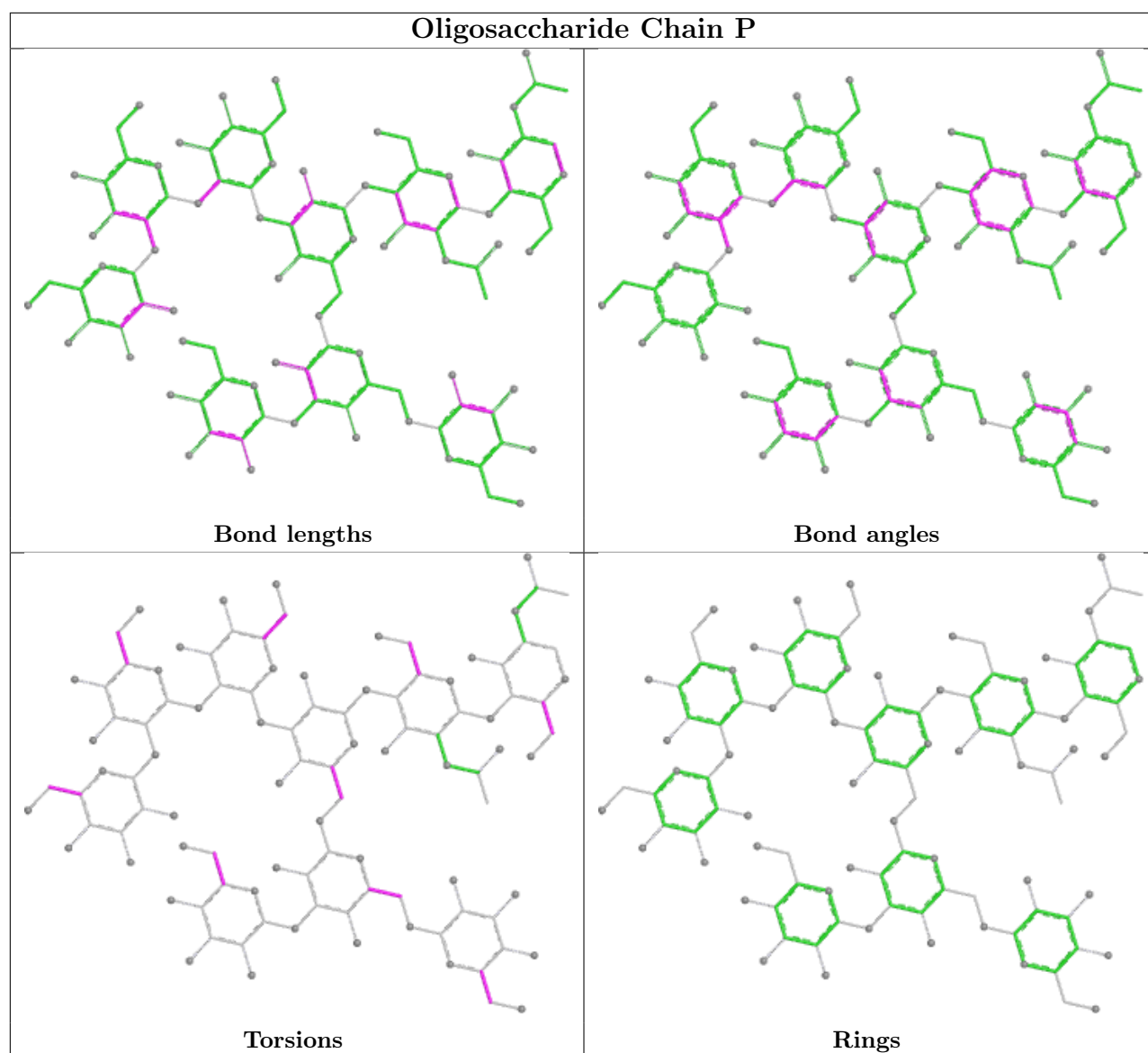


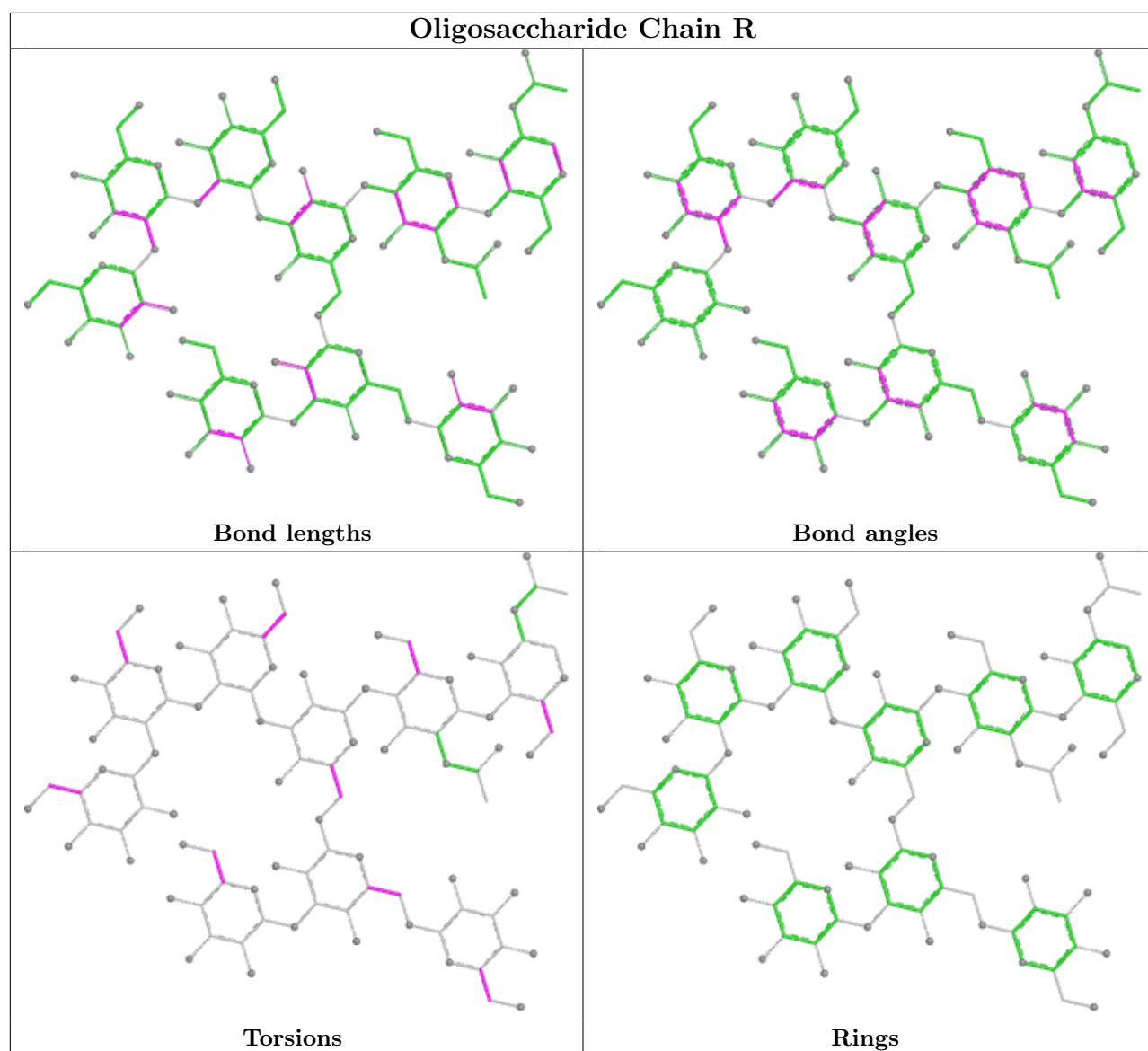


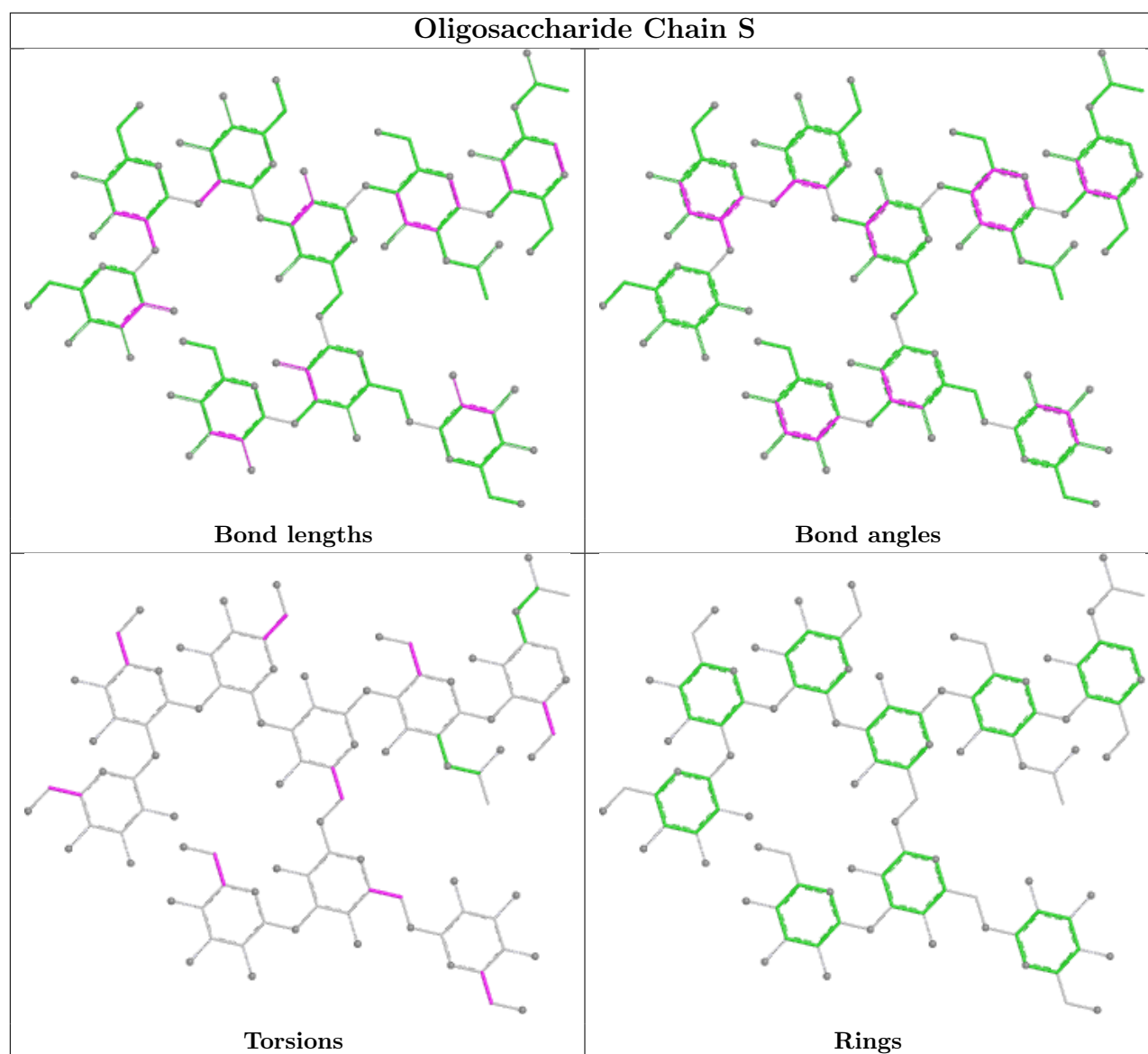












5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	1301	1	14,14,15	2.12	2 (14%)	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1301	1	14,14,15	2.12	2 (14%)	17,19,21	0.83	0
6	NAG	D	1301	1	14,14,15	2.12	2 (14%)	17,19,21	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
6	NAG	D	1301	1	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1301	NAG	O5-C1	6.67	1.54	1.43
6	C	1301	NAG	O5-C1	6.67	1.54	1.43
6	B	1301	NAG	O5-C1	6.67	1.54	1.43
6	D	1301	NAG	C3-C2	-2.56	1.47	1.52
6	C	1301	NAG	C3-C2	-2.56	1.47	1.52
6	B	1301	NAG	C3-C2	-2.56	1.47	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1301	NAG	1	0
6	C	1301	NAG	1	0
6	D	1301	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

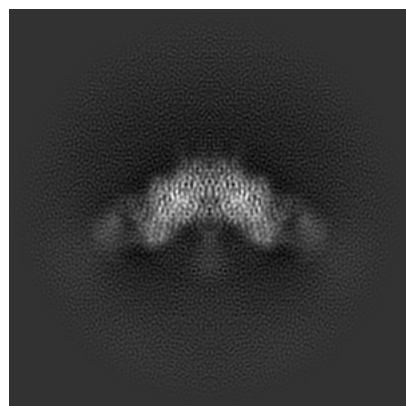
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20538. These allow visual inspection of the internal detail of the map and identification of artifacts.

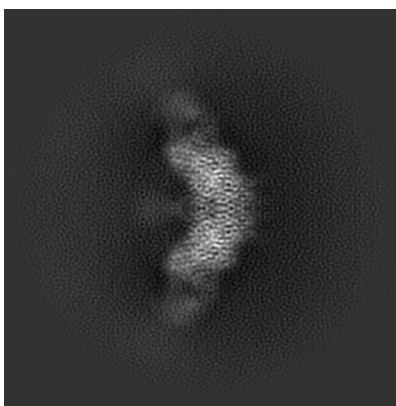
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

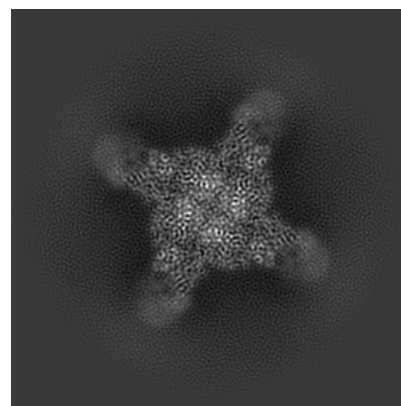
6.1.1 Primary map



X

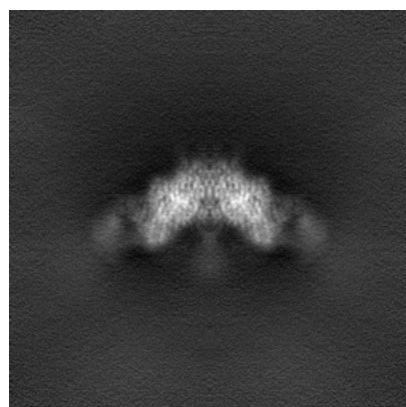


Y

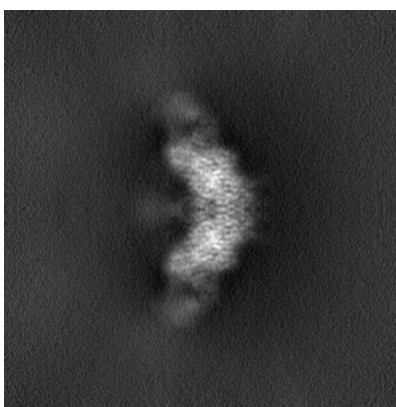


Z

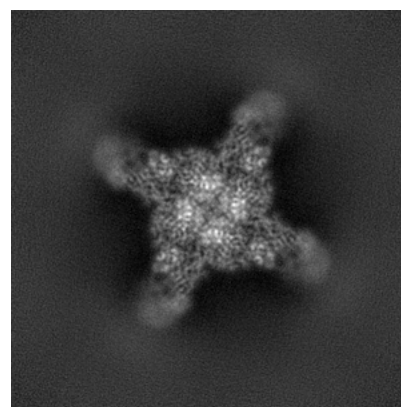
6.1.2 Raw map



X



Y

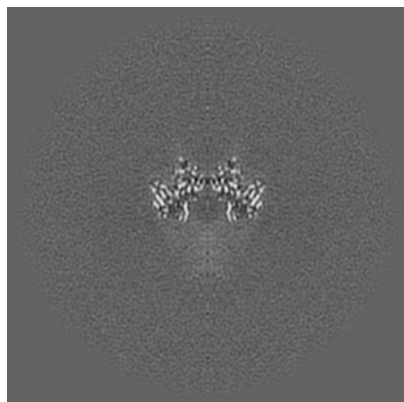


Z

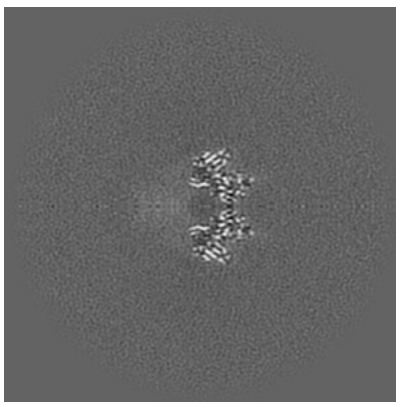
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

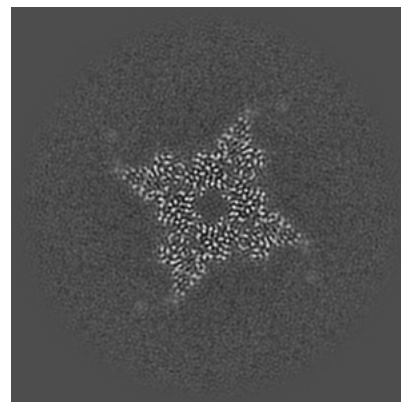
6.2.1 Primary map



X Index: 160

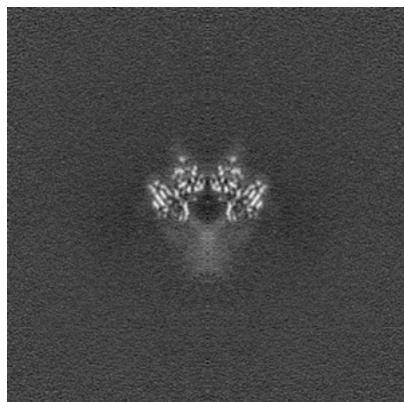


Y Index: 160

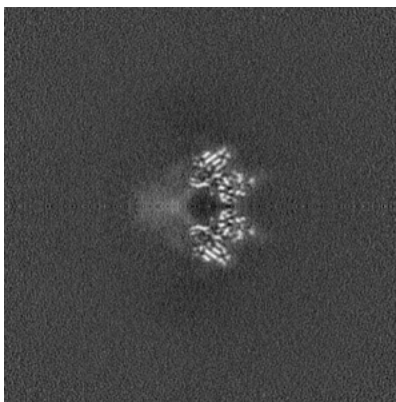


Z Index: 160

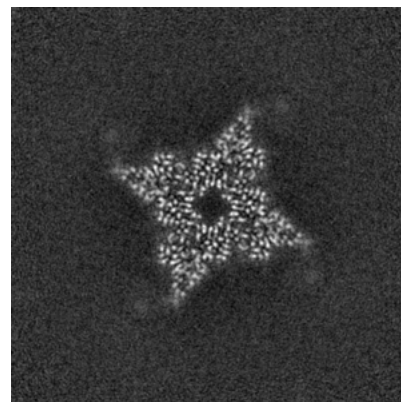
6.2.2 Raw map



X Index: 160



Y Index: 160

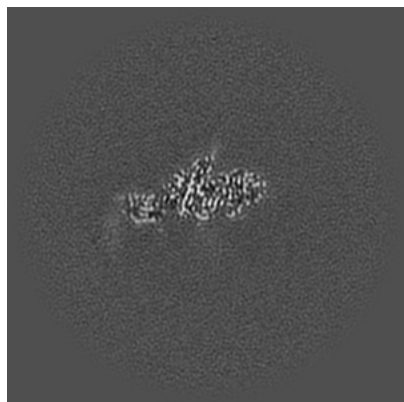


Z Index: 160

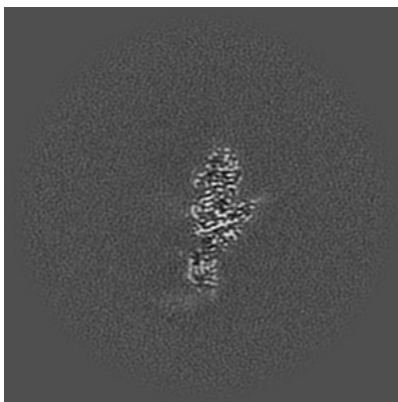
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

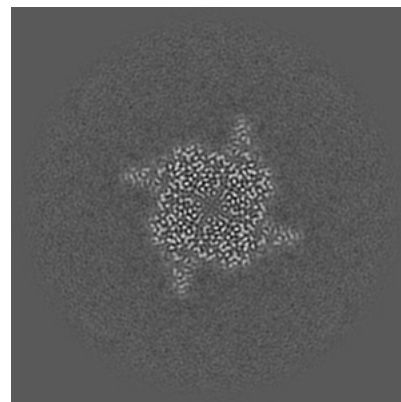
6.3.1 Primary map



X Index: 139

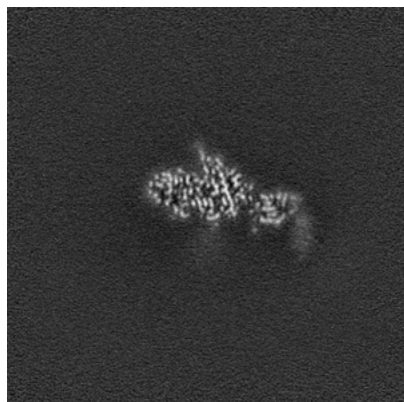


Y Index: 181

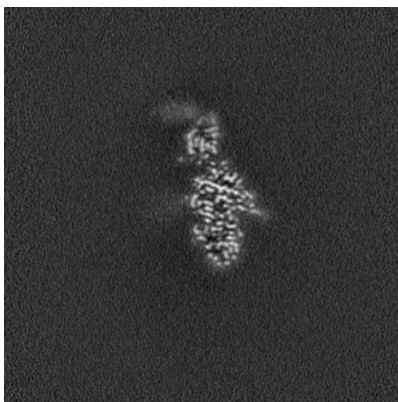


Z Index: 169

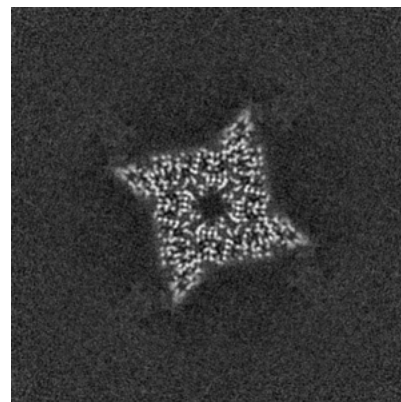
6.3.2 Raw map



X Index: 181



Y Index: 139

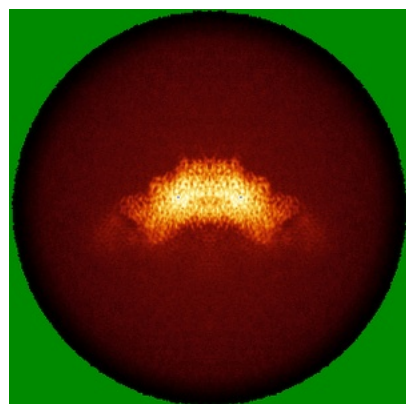


Z Index: 162

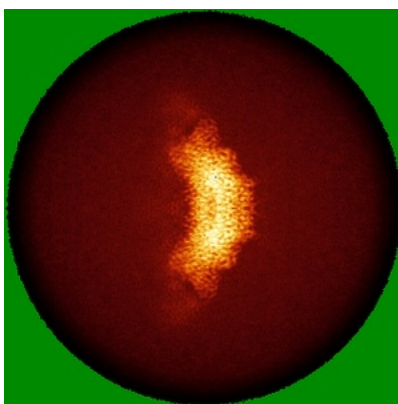
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

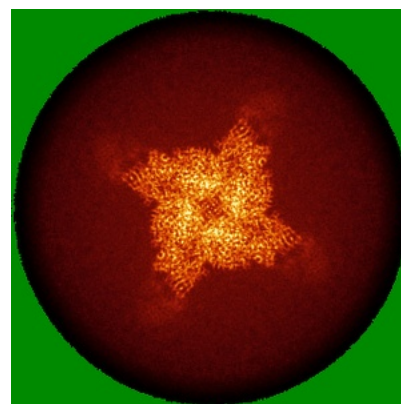
6.4.1 Primary map



X

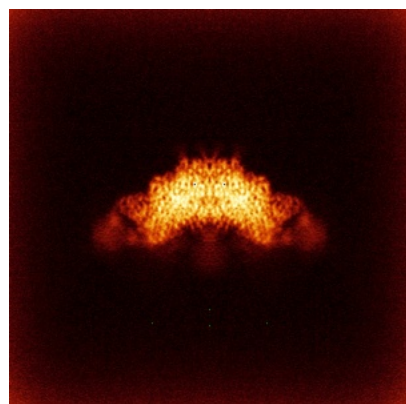


Y

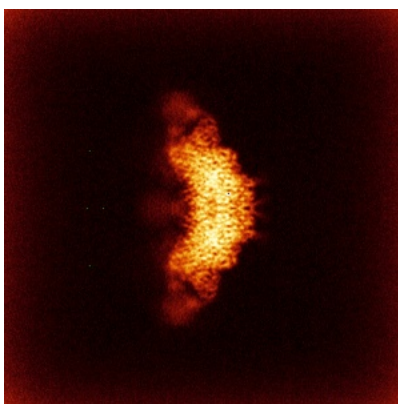


Z

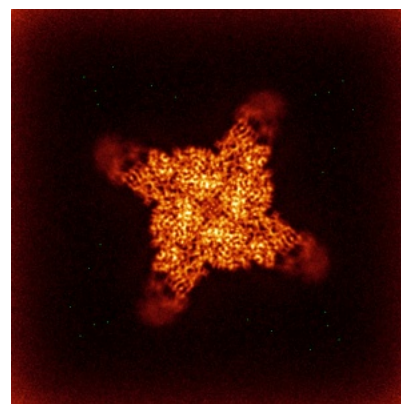
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

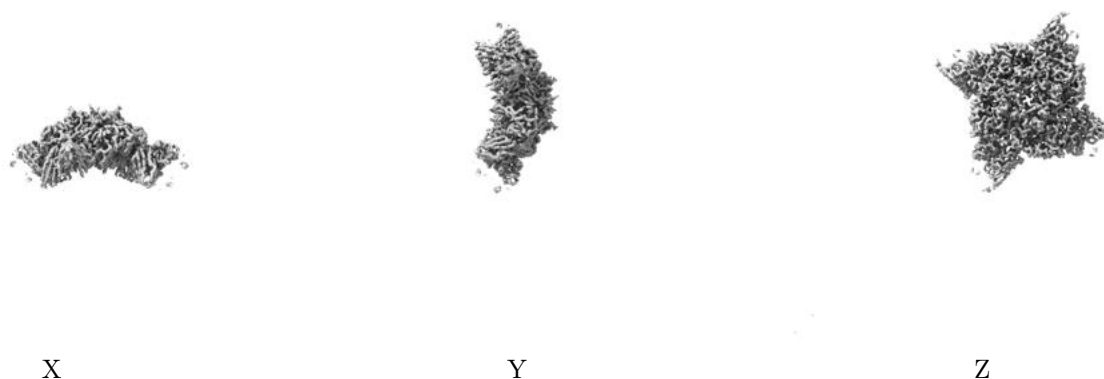
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.985. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

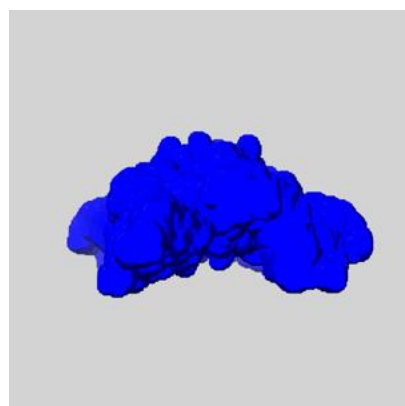
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

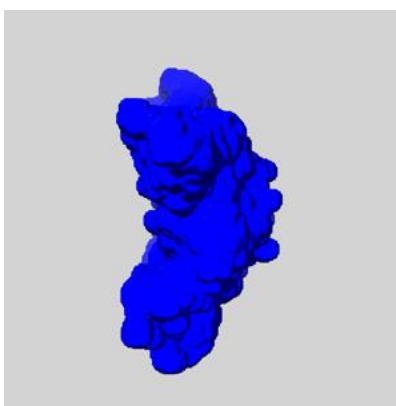
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

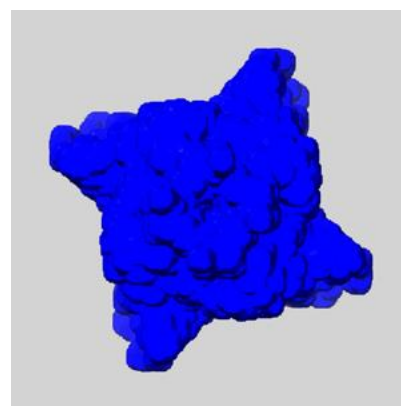
6.6.1 emd_20538_msk_1.map [i](#)



X



Y

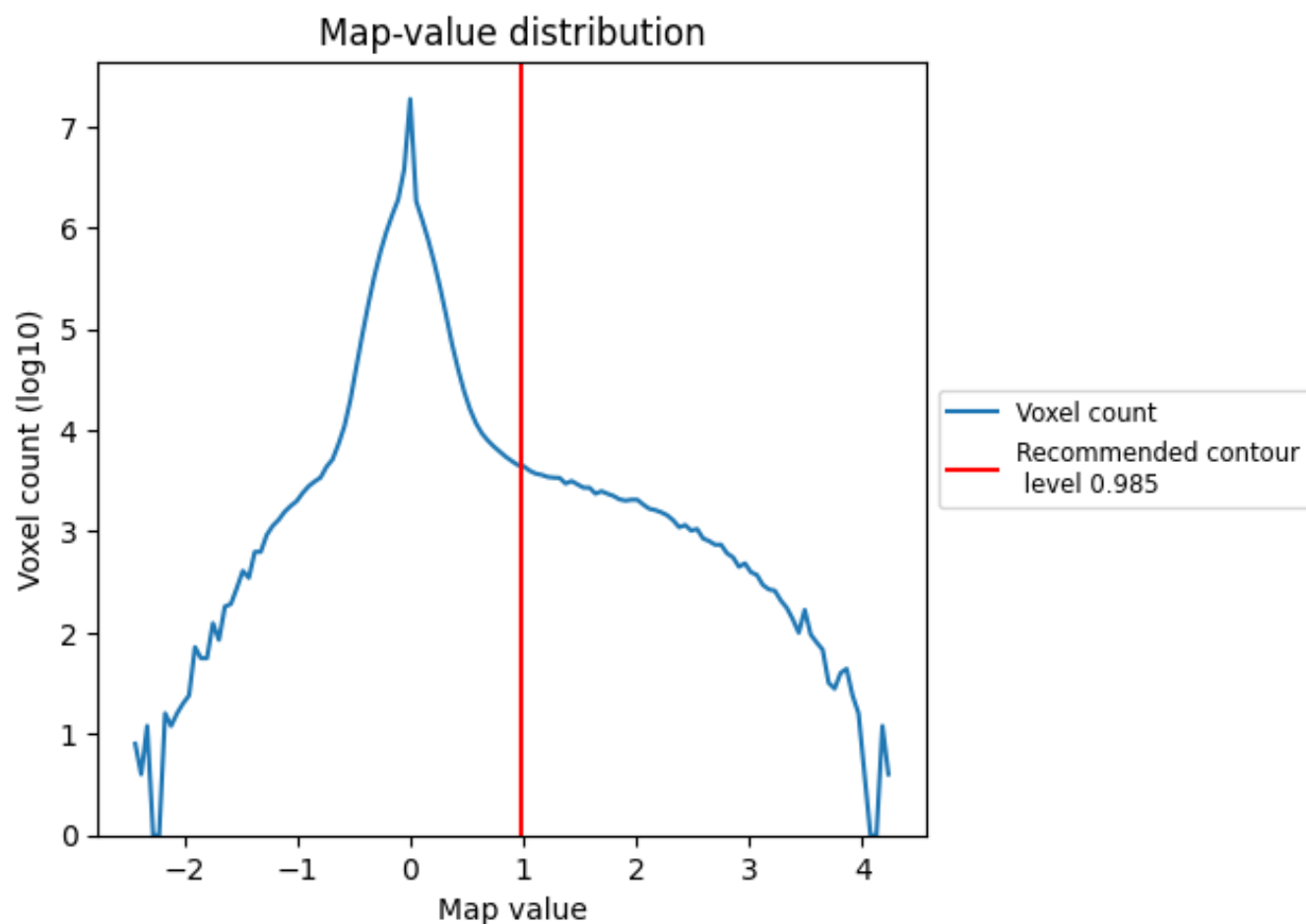


Z

7 Map analysis [i](#)

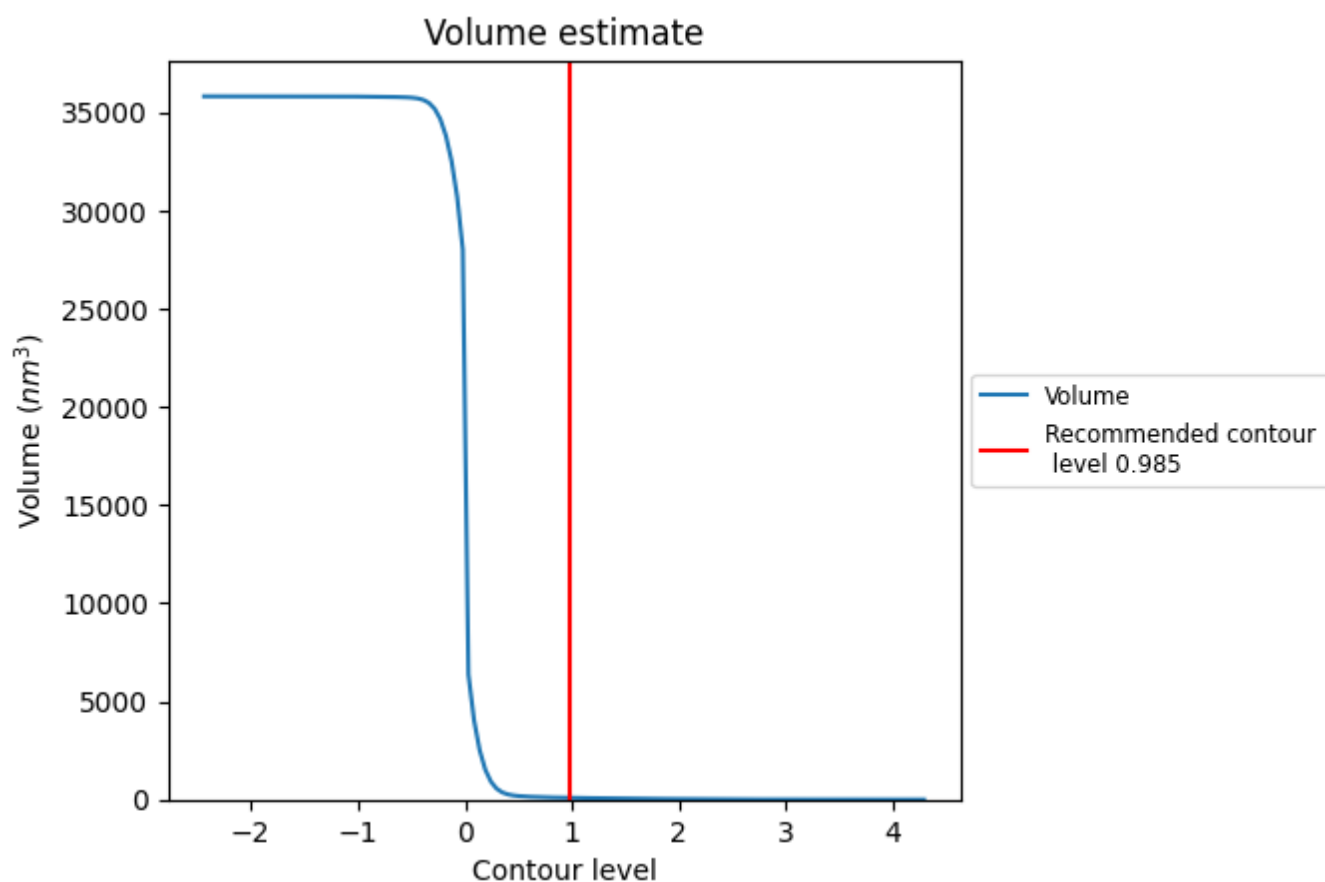
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

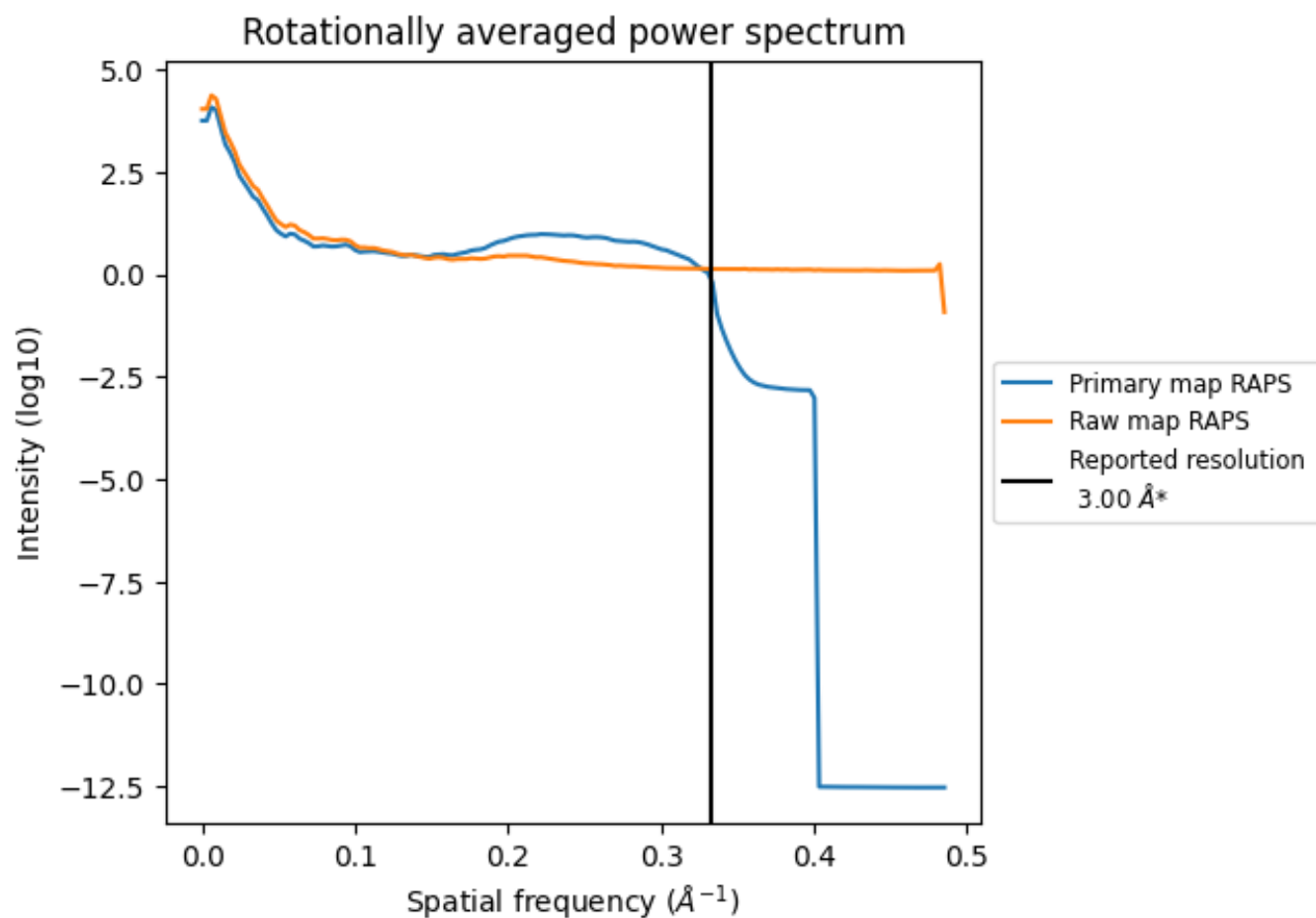
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 80 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

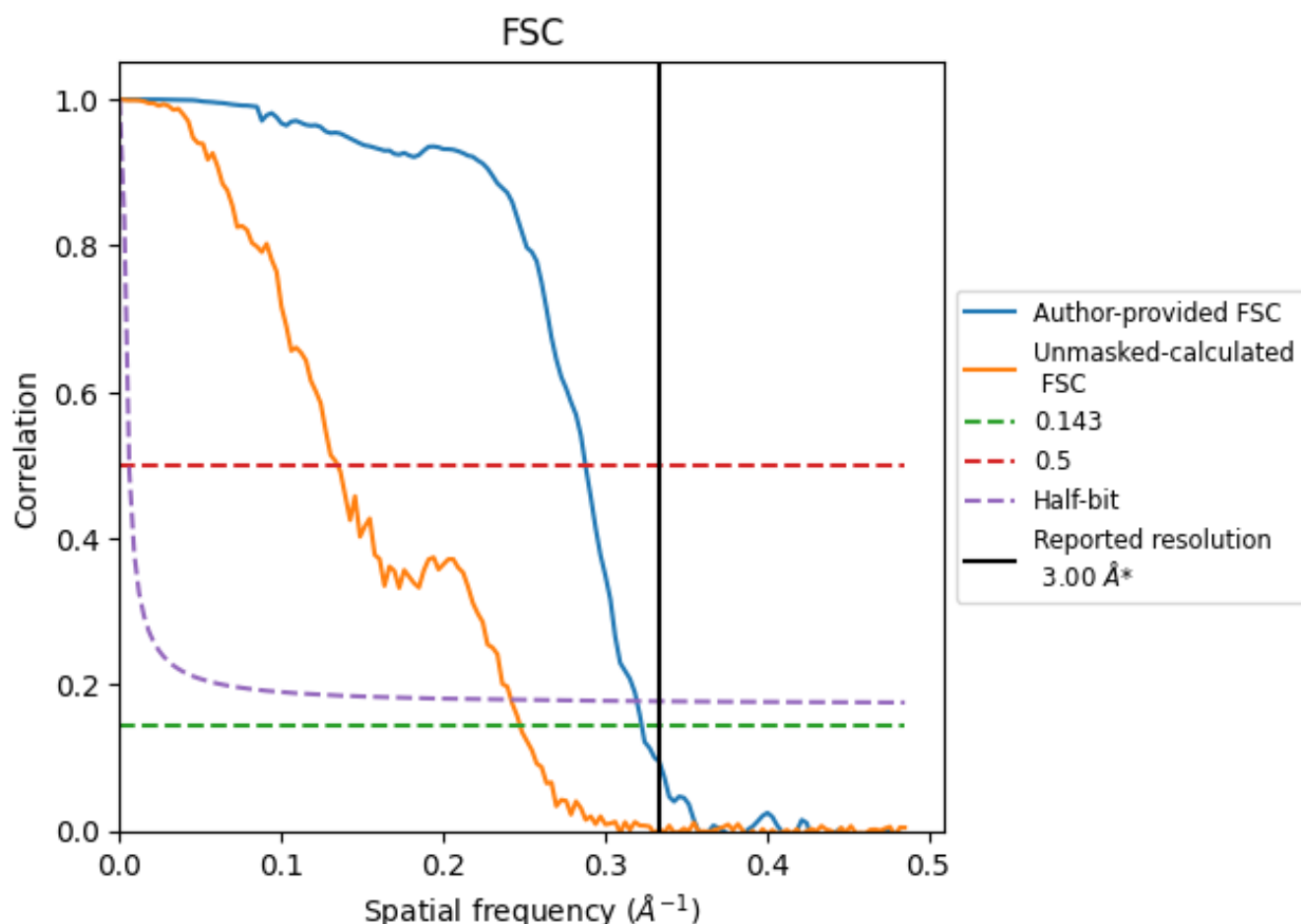


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

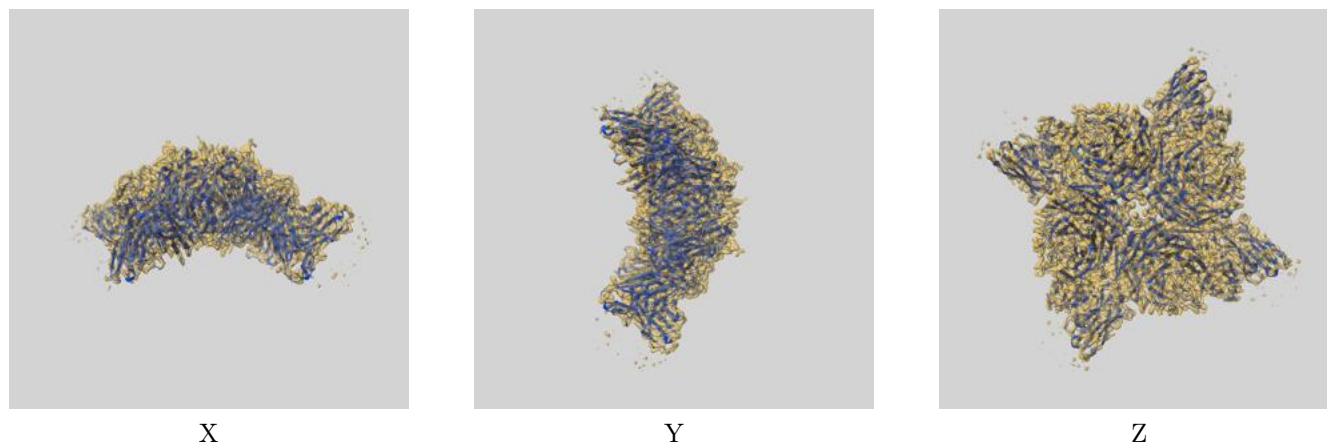
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.10	3.47	3.13
Unmasked-calculated*	4.04	7.42	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

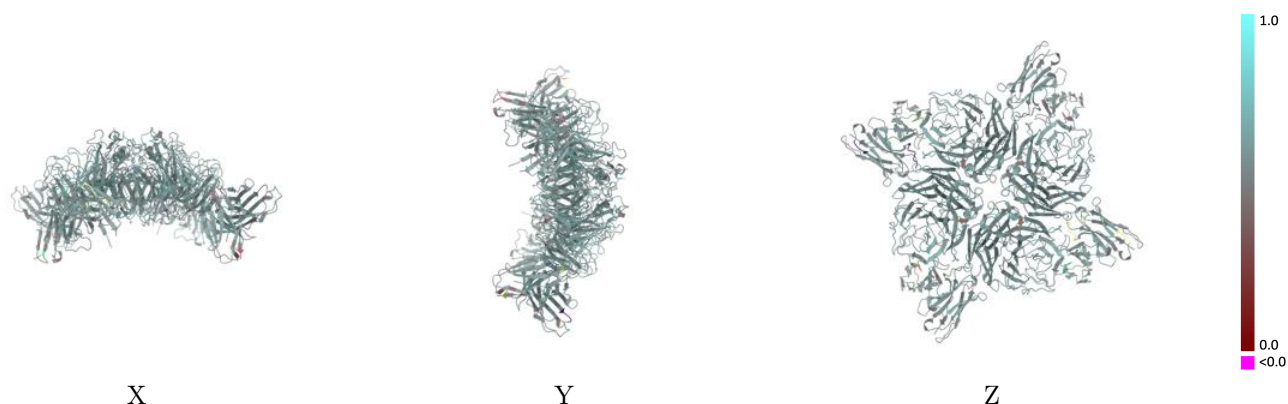
This section contains information regarding the fit between EMDB map EMD-20538 and PDB model 6PZW. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



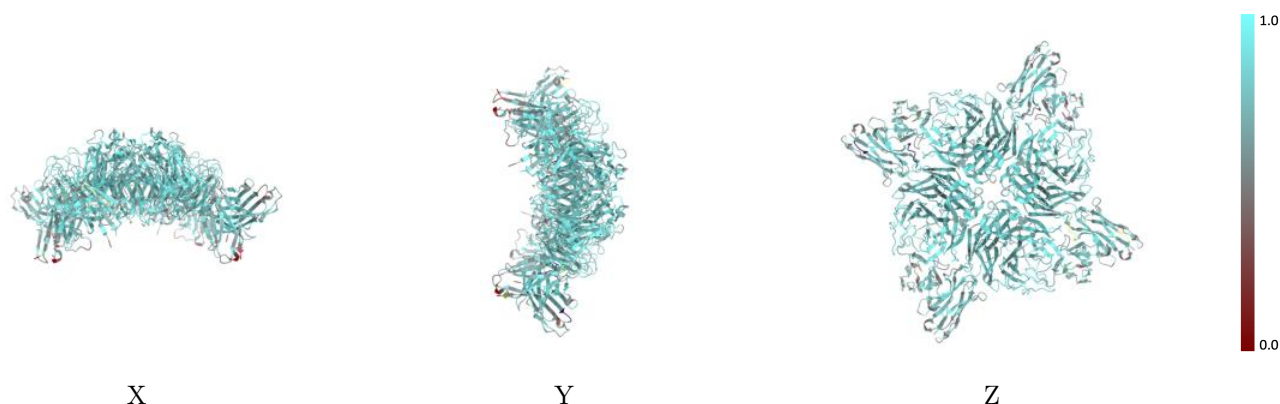
The images above show the 3D surface view of the map at the recommended contour level 0.985 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



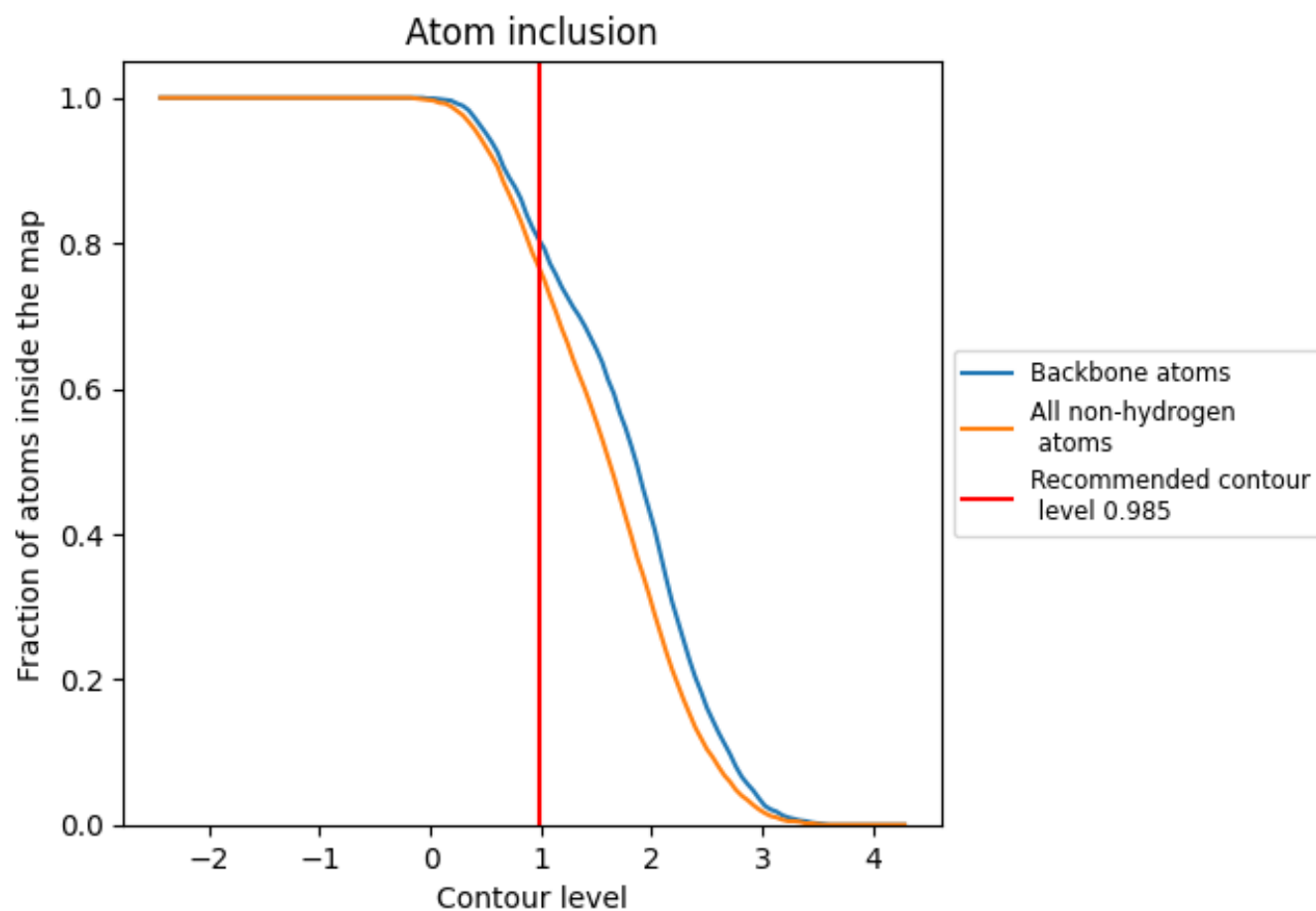
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.985).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.985) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5660
A	 0.8030	 0.5770
B	 0.8020	 0.5780
C	 0.8020	 0.5780
D	 0.8020	 0.5770
E	 0.6820	 0.5430
F	 0.7360	 0.5530
G	 0.6820	 0.5430
H	 0.7360	 0.5530
I	 0.6820	 0.5450
J	 0.7360	 0.5530
K	 0.7360	 0.5500
L	 0.6820	 0.5440
M	 0.5710	 0.5660
N	 0.6860	 0.5090
O	 0.5710	 0.5710
P	 0.6860	 0.5080
Q	 0.5710	 0.5610
R	 0.6860	 0.5160
S	 0.6860	 0.5160
T	 0.4640	 0.5520

